INDEPENDENT PEER REVIEW

OF

ANALYTICAL SOFTWARE TO SUPPORT INDUSTRIAL SUBTITLE D GUIDANCE

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June 28, 1999

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1.0 INTRODUCTION

The Municipal and Industrial Solid Waste Division of the U.S. Environmental Protection Agency's (EPA) Office of Solid Waste (OSW), in coordination with the Association of State and Territorial Solid Waste Management Officials Steering Committee and a Federal Advisory Committee Act group representing various industries, is developing guidance concerning the disposal of industrial non-hazardous wastes. The *Guidance* is intended to help state regulators and owners/operators of industrial facilities with non-hazardous waste to determine an appropriate site and design for a waste management unit (WMU). The *Industrial D Guidance* covers a variety of topics including: siting of WMUs, waste characterization, air controls, monitoring, groundwater protection, and corrective action. The *Industrial D Guidance* outlines a 3-tiered approach to the evaluation of a proposed WMU as it would impact groundwater quality. There are three levels of evaluation: 1) look-up tables based upon conservative assumptions and groundwater fate-and-transport analyses using a national database (Tier 1); 2) location-adjusted evaluating using an artificial neural network (Tier 2); and, a detailed evaluation involving site characterization and use of a site-specific groundwater modeling tool (Tier 3). Use of EPA's Industrial Waste Management Evaluation Model (EPAIWEM) is involved in Tier 1 and Tier 2.

The overall objective of the tiered approach to non-hazardous waste facility evaluation is to allow for differences in information and modeling needs from one facility to another. Specifically, one facility may wish to dispose of material with very low concentrations of a particular constituent while at the same time having very little information concerning the hydrology of the proposed site. Another facility may have a suite of chemicals that represent a range of leachate concentrations and have much hydrologic characterization data for the site. The tiered modeling approach is also intended to facilitate modeling by those who have little training in groundwater modeling, but understand the basic principles of hydrology. As a modeling tool, EPAIWEM is intended to address these differences in data and modeling capabilities among facilities. The *Guidance* and EPAIWEM are intended to facilitate discussion among state regulators, industry, and community environmental groups.

Prior to final release, a technical review of EPAIWEM, and the supporting documentation by those experienced in groundwater monitoring and neural network development was necessary to ensure that the methodology, the analytical approach, and the software tools were complete and appropriate for the intended purpose. The Economic, Methods, and Risk Analysis Division (EMRAD) in OSW tasked DPRA, Inc. to assemble a peer review team to conduct an independent peer review of the draft software and supporting documentation for the EPAIWEM, which will be released to states and industries as part of the *Industrial D Guidance* concerning appropriate measures for disposal of industrial wastes

Three peer reviewers with expertise in both groundwater modeling and neural network development and training reviewed the draft software and supporting documentation for the EPAIWEM. The panel included the following reviewers:

- Curtis Travis, PhD., Project Performance Corporation
- Donna Rizzo, PhD., Subterranean Research, Inc.
- Leah Rogers, PhD., Lawrence Livermore National Laboratory

In accordance with the Science Policy Council Peer Review Handbook (EPA 100-B-98-001), EMRAD prepared a specific Technical Charge to the peer reviewers which focused the peer reviewers on specific issues in each of their areas of expertise, as well as on the general layout of the document. Each reviewer prepared a letter/memorandum report which documented their review efforts and comments.

This report collects and summarizes the comments received from the peer reviewers into one comprehensive document. The report is organized into four sections including: Section 1.0 - Introduction, Section 2.0 - General Issues, Section 3.0 - Specific Responses to Technical Charge Questions, and Section 4.0 - Conclusions. Please note that this report does not provide a full set of the original review comments prepared by the peer review panel. The original comments submitted by each reviewer are attached to this report as Appendices A - C. The appendices present the original comments of the peer review panel in their entirety, including marginal comments on supporting documentation where provided.

2.0. GENERAL ISSUES

Overall the reviewers found the tiered approach presented in the *EPA Industrial Waste Evaluation Model* (EPAIWEM) to be very useful in for evaluating WMU designs. The panel felt, in particular, that the model would help those facility owners/operators, as well as state and local staff, with less experience in ground water modeling. The software and graphical interface were praised for ease-of-use and clarity. The reviewers also uniformly and positively commented on the usefulness of the well-written and user-friendly supporting documentation. Each reviewer made general comments about the EPAIWEM, including general comments on the development and training of the artificial neural network (ANN). These general comments are summarized below.

All of the reviewers found the EPAIWEM software and its underlying models to be high-quality, technically-sound work; however, one reviewer had serious misgivings about the overall organization and redefinition of standard ANN terminology in the Technical Background Document (TBD). This reviewer provided in-depth, specific comments on suggested improvements to the TBD to improve the quality of the TBD and, as a result, the underlying Tier 2 ANN model. The other two reviewers, while not explicitly stating their concerns with the TBD in general, did provide many specific comments which reflected that viewpoint. In most cases, reviewers commented on the discussion presented in the TBD, and how that discussion could potentially affect a user's understanding of the EPAIWEM's underlying models. Please note those references to page numbers throughout Section 3, refer to specific pages within the TBD.

The reviewers found that the use of EPA's Composite Model with Transformation Products (EPACMPT) and it Monte Carlo adaption to compute probabilistic estimates of constituent concentrations in groundwater is appropriate. The probabilistic approach allows for quick screening of sites using a minimum amount of site-specific data, which will save users time and money.

Reviewers found that the ANN training and testing demonstrate that ANNs can reasonably predict the general pattern of the EPACMPT model results over a range of input parameters. However, contradictory results and recommendations, problems with the neural network training, and the non-intuitiveness of the input parameters decrease confidence in the code and the ANNs predictive capability. One of the difficulties is that there are too many input parameters used in the construction of the neural networks. In addition, one reviewer felt that some important parameters, such as groundwater flow rate, were omitted. These comments are more thoroughly discussed in Section 3.3 The Quality and Appropriateness of the Artificial Neural Network Tool.

For a summary of the specific comments related to the questions raised in EPA's Technical Charge to Peer Reviewers, please see Section 3.0.

3.0 SPECIFIC RESPONSES TO TECHNICAL CHARGE QUESTIONS

The Technical Charge to Reviewers developed by EMRAD requested that the technical peer review panel focus on four major areas in reviewing the EPAIWEM software and accompanying documentation. Each of these major review areas is presented in the following Subsections:

- Section 3.1 -- The Application of EPACMPT to the Tier 1 and Tier 2 Analyses;
- Section 3.2 – The Assumptions and Parameters Used to Develop the Tier 1 and Tier 2 Evaluations;
- Section 3.3 -- The Quality and Appropriateness of the Neural Network Tool for its Intended Purpose; and,
- Section 3.4 -- The Overall Quality of the Software and Documentation.

In each of these areas, the Technical Charge directed the peer review panel to provide comments on very specific areas. These specific directions and the peer review panel responses are provided below. For purposes of clarity, the specific direction provided by EMRAD is presented in italics immediately followed by a summary of the reviewers' comments.

3.1 The Application of EPACMPT to the Tier 1 and Tier 2 Evaluations

Reviews of EPACMTP by the SAB and other independent peer-review panels have focused on the assumptions, approaches to sampling, and the computational methods. This review is not intended to be a review of EPACMTP, per se, but instead a review of its application to the development of IWEM.

- *Comment on the tiered approach to analysis of the WMU liner-design. Does it serve the intended purpose?*

All three reviewers found that the tiered approach to analysis of the WMU liner-design was reasonable and met its intended purpose. One reviewer stated that "The tiered approach was designed to accomplish two objectives: (1) allow for the two cases of sites with very little information concerning hydrology and for sites with a much more complete characterization of ground water hydrology, and (2) facilitate modeling by those with little training in ground water modeling. The two-tiered approach presented in the document accomplishes both objectives. The two-tiered approach is reasonable in that it permits users with varying degrees of site characterization data to obtain an immediate analysis and recommendation. Those with little site-specific data can use EPACMTP model results based on national-level data that will result in leachate concentration threshold value (LCTVs) that would be protective anywhere in the nation. Those with more site-specific data can input the data into the appropriate neural network and obtain more site-specific LCTVs."

- *Given the assumptions for the Tier 1 evaluation, is EPACMTP an appropriate tool to use? Are the results appropriate for the type of analysis?*

Each reviewer found that the EPACMPT is an appropriate tool as applied to the development of the EPAIWEM. One reviewer specifically commented that the "EPACMTP is a state-of-the-art ground water fate and transport computer code that has received extensive peer review by the EPA Science Advisory Board and other review committees. It simulates one-dimensional, vertically downward flow and transport of contaminants in the unsaturated zone as will as two-dimensional or three-dimensional groundwater flow and contaminant transport in the saturated zone. Probability distributions of input parameters were obtained from a nationwide survey of industrial non-hazardous Waste Management Units and their surrounding hydrogeologic characteristics. EPACMTP accounts for chemical and biological transformation processes and is capable of determining overall decay rates from chemical-specific hydrolysis constants using soil and aquifer temperature and pH values. We believe that given the extensive peer review that EPACMTP has undergone and its previous widespread application by EPA, the current application of EPACMTP as the basis for EPAIWEM is appropriate."

- *Is EPACMTP an appropriate tool for generating the response surfaces modeled by the artificial neural networks? Is there another tool or modeling approach that would serve the purpose of the Tier 2, location-adjusted evaluation?*

All of the reviewers found that the EPACMTP is an appropriate tool, run in Monte Carlo mode. No reviewer suggested an alternative tool or modeling approach that would better serve the purpose of the Tier 2, location-adjusted evaluation.

3.2 The Assumptions and Parameters Used to Develop the Tier 1 and Tier 2 Evaluations

- *Comment on the assumptions and parameter ranges used for developing the Tier 1 National Evaluation. Are the assumptions appropriate for the type of analysis? Are the parameter ranges reasonable?*

Each of the reviewers found, in general, that the assumptions and general categories of parameters used for developing the Tier 1 evaluation were reasonable and appropriate. However, one reviewer had specific comments on individual parameters, or categories of parameters used in the Tier 1 evaluation. Several of these comments are summarized below; however, to gain a complete understanding of the reviewer's concerns, readers should consult the original peer review comments.

The reviewer indicated that the time period (10,000 years) over which contaminant migration is modeled is unduly long and suggested that current models cannot produce accurate results over this time period.

Chemical-specific biodegradation rates are not included/discussed as sensitive parameters. It is not clear if any biodegradation rate was assumed in the EPACMPT Tier 1 and Tier 2 calculations. In addition, the median and range of decay rates are not discussed in the TBD text, but decay rates are presented in TBD tables. This should be clarified.

The reviewer wanted to see a discussion of the relative importance of dispersion, dilution, and degradation in the computation of the dilution/attenuation factor (DAF). The reviewer felt this would help the user determine if site-specific biodegradation data would be useful in a Tier 3 analysis.

The reviewer questioned the use of hydrous ferris oxides values in the modeling. The reviewer stated "Hydrous ferric oxides will tend not to be found in reducing groundwater environments which constitute a large proportion of sites. This method for determining K_d values seems best applied on a site-specific and not on a national tier 1 analysis."

The reviewer also questioned the assumption that the leachate pulse duration is the same as the operating unit's life. The reviewer stated that leachate will continue to migrate from the operating unit after the assumed operating unit's life and that the assumption that remaining waste is either removed or has negligible additional contribution to leachate is not conservative and is unrealistic.

- *Comment on the approach to estimating infiltration for the various WMUs and liner designs. Is the use of regional climatic data sufficient to generate appropriate ranges for the no-liner and single clay liner scenarios? Are the assumptions used for developing the infiltration rates for the no-liner, single clay liner and composite liner appropriate and realistic? If not, please recommend other assumptions or approaches to estimating infiltration. Is there a way to modify the approach to determining liner- dependent infiltration rates in a way that balances long-term liner failure with the efficacy of long-term liner maintenance?*

In general, the reviewers had no issues with the overall approach(es) for estimating infiltration. No comments were received on the adequacy or inadequacy of the use of regional climatic data. However, two reviewers had issues with some of the assumptions used for developing infiltration rates for liners. These reviewers provided comments that would slightly modify the approach to calculating infiltration rates.

One reviewer assumed, that the infiltration rate is the most sensitive of the input parameters used in EPACMPT. The reviewer felt that the TBD should document the choice of the range of infiltration rates given in Table 4-1, 4-2, and 4-3 for the no-liner and single-liner scenarios and should also explain the differences for these rates in the tables for landfills, surface impoundments, and Waste Piles. The reviewer also questioned why the infiltration rate for the surface impoundment composite liner (Table 4-2) is less than the infiltration rates for composite liners in Tables 4-1 and 4-3 since infiltration rates for no liner and single liner in Table 4-2 are larger than the corresponding infiltration rates in Tables 4-1 and 4-3.

One reviewer questioned the assumption of a single leak per acre for calculating infiltration rates in composite liners. This reviewer felt that a more consistent (with the rest of the modeling) would be to sample a range of geomembrane leakage rates using actual data from studies (e.g., Darliek et al., 1989) as opposed to a single leakage rate. This would be more consistent with the Monte Carlo sampling of a range of values used for other parameters.

One reviewer felt that the TBD does not clearly explain, in Appendix B, how Rip/Tears are treated in calculating infiltration rates. This reviewer also felt that the use of three soil types do not adequately represent what is found in nature -- the soils chosen do not address soils that are essentially sands or clays.

One reviewer felt that the TBD should include a brief summary about what types of clays are recommended to reach the 1 x 10 -7 cm/sec hydraulic conductivity levels, how difficult it is to insure an even 3-ft layer, or other interesting issues about quality and consequences of liner construction.

- *Comment on the parameters used for the Tier 2 Location-adjusted Evaluation. Are the parameters appropriate to the type of analysis? Are they parameters that would generally be known about a site? Should more parameters be included? If so, which ones? Should parameters be deleted?*

One reviewer felt that the use of seven parameters in the Tier 2 analysis is inappropriate. The reviewer noticed that the ANN predictions have a scatter round the baseline model predictions. This reviewer felt that the observed scatter could be reduced by combining selected input parameters based on the important physical processes the system is representing.

The reviewer also noticed an anomaly with the reduction of the parameters from 12 to 7. An organic carbon partition coefficient (Koc) was listed as one of the seven parameters but there was no associated organic carbon number. Organic carbon numbers were dropped in moving from 12 to 7 parameters. In a mechanistic sense, one needs an organic carbon number to be able to use a Koc. In a probabilistic sense, the higher Koc values will produce more retardation than lower Koc values.

The reviewer felt that a possible solution for the EPAIWEM neural network would be to group selected parameters together so that the total number of training parameters is reduced. For example, combining the surface area and infiltration rate defines the mass flux of chemical to groundwater which should be one of the most important parameters in predicting down-gradient concentrations. Please see the original peer review comments for specific suggestions of how to group/modify parameters to improve results.

One reviewer had great difficulty with the following statement on page A-7. “Modeling the landfill scenario with EPACMTP assumes an essentially steady-state scenario in which the organic carbon partition coefficient (KOC) has little or no effect on the output. Therefore, the landfill neural network did not consider KOC as an input parameter and did not use the average peak 30-year concentration as an output parameter." This reviewer questioned how a steady-state scenario with KOC having little or no effect on the output justified the elimination of one of the ANN output parameters (max 30-yr ave. well conc.). The reviewer questioned whether this output parameter eliminated due to complications in training and requested clarification within the document.

3.3 The Quality and Appropriateness of the Artificial Neural Network Tool

In training the ANNs, parameter values that ranged between the 10th and 90th percentile of the parameters distribution were used. Consequently, the ANNs were not trained in the range of infiltration rate assumed for the composite liner (3×10^{-5} m/yr). The resultant error between EPACMTP and the ANNs when using the composite liner infiltration rate was considered unacceptable. Thus, the composite liner scenario is not included in the Tier 2 evaluation for this draft of IWEM.

[Note: peer review comments in Section 3.2, often overlapped between specific issues raised in the technical charge. This summary document has sorted these types of "overlapping" comments under one technical charge issue. Please see the original peer review comments for the original flow and organization of comments.]

- *Comment on the overall approach to developing the neural networks. Was the program used for training the ANNs appropriate?*

In general, reviewers found that four difficulties arise with the development of the neural networks: (1) incorrect design of the neural network, (2) too many input variables in the neural network (3) inappropriate training of the neural network, or (4) too large an error between the neural network predictions and output of the EPACMTP model. The reviewers provided comments for each.

One reviewer felt that the TBD did not clearly, and/or accurately in many cases, explain definitions and terminology used to describe the Tier 2 ANN. The reviewer believes the selected algorithm to be appropriate for training.

The Tier 2 neural networks were developed using a single hidden layer. Although a neural network with a single hidden layer and N-1 nodes is theoretically capable of approximating any response surface with N patterns, this type of neural network may be very difficult to train. There is no way to tell *a priori* whether or not one or two hidden layers will give the best results. Simple response surfaces can be fit easily with a single hidden layer; more complex surfaces require two hidden layers to obtain good fits. The response surface of the EPACMTP model is fairly complex. It is a nonlinear function with response surface spanning several orders of magnitude. Since distributions of the input parameters were not specified in the documentation, it is not clear if the EPACMTP function is defined on a compact set; if not, the problem is even more complicated.

Thus, it may be that more than one hidden layer is required to approximate this surface with minimal error.

One reviewer felt that the Tier 2 neural networks have too many input variables. Reducing the number of input variables will speed up training and decrease the prediction error.

Reviewers felt that the TBD was not clear on what combination of training was used to train the Tier 2 neural networks. For example, both Back Error Propagation and the conjugate gradient method were used to train the neural networks. However, page 55, Paragraph 3 of the TBD implies that only conjugate gradient was used in training. Documentation needs to be clearer on what combination of training was used to train the Tier 2 neural networks,

The optimal learning rates of neural networks often changes dramatically during the training process. Page A-15 states that the learning rates for the Tier 2 neural networks were not modified during training. Training a neural network using a constant learning rate is usually a tedious process requiring much trial and error.

One reviewer felt that the TBD should provide some justification for selecting the method of backpropagation (specifically NNModel version 3.2). Although backpropagation is the only ANN algorithm provided by Neural Fusion (1998), other algorithms exist that would have greatly simplified the lives of the developers. If one of the goals was to find an algorithm that would approximate processes in the same manner as regression analysis, then EPAIWEM developers may want to consider the General Regression Neural Network (GRNN) in a second-generation model. The GRNN algorithm has its theoretical foundations in regression analysis and requires very little training time. If the developers choose to remain with backpropagation, the developers could implement modular ANNs in a second-generation model (*i.e.*, have separate ANNs for ranges of data where the training patterns appear to compete with each other). This would help the predictive capability of the backpropagation networks and greatly reduce training times.

The reviewer took exception to the statement (page A-29) that "In general, the neural network predictions for input parameters outside the 10th to 90th percentile values will likely be less accurate than for input values within this range." The reviewer states that the neural network should not really be used to predict values in a range that it has not been trained on. The reviewer comments that if the ANN must make predictions outside the 10th to 90th percentile range, then a second-generation model should include separate ANNs that are trained on data in each of these ranges (0 to 10 and 90 to 100). Another reviewer commented that the decision to generally train and validate the neural networks using input values in the range of 10^{th} to the 90^{th} percentile. This is a serious problem with the training protocol for the neural networks.

The reviewer also commented that principle component analysis of the data should be conducted before selecting the subset of input parameters. This would help justify why the backpropagation network did not perform well, when all 10-12 input parameters were considered, and identify additional regions of the input parameter space in which to modularize the ANNs.

The TBD states that “overfitting”of neural networks can be avoided by careful choice of neural network size and the amount of training applied to the neural network. Reviewers felt that this statement is incorrect and felt that the TBD may include a discussion of how the training set is usually such a small sampling of the overall range of possibilities or search space and overfitting is where network weights get too specialized on idiosyncratic features of the training set and thus has a lower generalization performance (i.e., performance on the larger search space beyond the training set).

One reviewer felt that a serious omission in the TBD’s documentation of the neural network development is how the necessary one-to one correspondence between neural network input parameters and the EPACMTP model output was established. In particular, the document is not clear on how the correspondence between the neural networks deterministic input parameters and the 90th percentile DAF computed by EPACMTP is established.

One reviewer felt that, throughout the TBD, the authors confused the terms “training” data sets, “test” data sets, and “validation” data sets. The reviewer felt that a reader of the TBD was never told which of these “training/test/validation” data sets were used to train the neural networks used in the IWEM (*i.e.*, used to fix the weights of the ANNs before they are used for validation and/or predictions). This could lead to misunderstanding/mistrust of the ANNs. (Please see the original peer review comments for comments on specific pages within the TBD.)

- *Comment on the number of parameters, the range of values, and the combinations used for training. Is there a training method or approach that would enable inclusion of parameter values span many orders of magnitude?*

Reviewers noted that the TBD text states that twelve parameters were selected to develop the neural network but 13 parameters are listed in Table 3-7.

One reviewer commented that dimensional analysis of the geometric, flow, and chemical parameters that govern the model prediction of the DAF may be a useful tool to augment or enhance the training data sets for the ANN.

The reviewers felt that, given that many state regulations require a groundwater resource protection standard along with protection of existing supply wells, it may be more appropriate to use a training data set for the ANNs which places the well directly in the centerline of the plume. This may make the final IWEM results more compatible with typical regulatory decision processes. In addition it may provide a training data set which covers fewer orders of magnitude and allows the ANNs to achieve a better fit to the response surface.

One reviewer felt that the developers of the EPAIWEM may wish to reconsider the deletion of two of the parameters removed from the original list of parameters used to develop the ANNs, the Darcy velocity and the angle of monitoring well off the centerline of a plume.

- *Comment on the overall quality of the ANNs as described by the various criteria used. Are there other criteria that should be used to evaluate the quality of the ANNs? Is the error between EPACMTP and the ANNs acceptable in the context of the uncertainties associated with groundwater modeling?*

Overall, the reviewers felt that the criteria used, such as R^2 values, plot, histograms, etc. were appropriate, and that the quality of the ANNs is high. However, one reviewer questioned how the data transformations have affected the evaluation of the ANNs effectiveness using the criteria. For example, the coefficient of determination, R^2, will be increased by using log-transformed data. It is unclear whether the predicted and measured concentrations would have exhibited an R^2 that met the stated acceptance criteria (R^2 of 0.9) without manipulating (transforming) the data.

One reviewer found that running the code produced contradictory results and recommendations. For example, in certain situations the Tier 2 analysis resulted in higher DAFs for the No Liner scenario than for the Single Liner situation. Because of this, depending on initial leachate concentrations, a chemical would be protective without a liner and not be protective with a liner. In other words, a higher LCTV was achieved under the No Liner than with the Single Liner Scenario. These results contradict reality and diminish confidence in code's predictability.

- *Comment on the various approaches used to filling in the response surface for the purpose of getting a better fit between EPACMTP and the ANNs. Is there a method for better incorporating the extremes of the parameter distributions?*

Only one reviewer specifically commented here. The reviewer felt that one of the biggest limitations of the code is the assumption of homogeneity in aquifer stratification (thickness). Currently the model training data sets use a 90th percentile of the aquifer thickness in the range 80 to 90 meters -- the reviewer states that most contaminant plumes are confined to layers which are on the order of 3 to 10 meters thick. This observed plume distribution is presumably the result of aquifer heterogeneity which typically is not represented in most groundwater modeling applications. In order for the DAF factors to be conservative it may be prudent to consider limiting the aquifer thickness to a typical range of plume thicknesses that have been observed in many cases (i.e., artificially force the model results to limit the plume thickness by constraining the aquifer thickness).

- *Comment on the approaches to selecting the training, test, and validation data sets.*

One reviewer stated that the EPAIWEM used state-of-the-art methodologies to emulate the output from the EPACMPT code. The tools it used in conjunction with the methodology appeared to be well thought out and appropriate. The intended purpose was met in that a high degree of correlation was obtained between the EPACMPT outputs and the predictions made by the IWEM model.

One reviewer felt that the discussions of the how the testing and validation data sets relate to each other and if there is any overlap between them should be clarified. In addition, the reviewer wanted to see more landfill and land application training data sets, as well as, more training to gain in predictive ability.

The reviewer felt that the TBD would benefit from a more complete discussion of the logic behind the creation of additional data samples. For example the group 1 data samples appear to be created to add in test data which had not been well predicted by the networks (i.e., higher residuals) to the training data. The discussion of the Group 4 data samples is good Overall one has the sense from the conclusions here that the waste pile and land application unit networks benefitted from what you learned during training the landfill and surface impoundment nets and the former two nets have better summary statistics (pg. 62). It is not clear that you took all that you learned back into the training of the landfill and surface impoundment nets to get the best performance you could from them.

Another reviewer felt that the process for selecting the training data set for training the neural network does not appear to be optimal. The current approach is to choose equal frequencies of values over regular increments of input values (Page A-9, Paragraph 2). However, this procedure will result in an over representation of infrequent values when training a neural network over the range of the distributions of the input parameters. The reviewer feels that it is more reasonable to use a Latin Hypercube procedure, which selects samples relative to their frequencies, to sample the input parameter distributions to construct the training data set.

One reviewer stated that the histograms of input values used in training (Figures A.2.6 and A.2.7) do not appear to show equal frequencies for each value over the range of values -- that too much emphasis is placed on using the pure “star-point” distributions. The reviewer believes that, if obtaining equal frequencies for the training input values is deemed important, training input values should be selected by sampling randomly from a uniform distribution of the range of input values.

The reviewers felt that the neural network predictive capability would be improved through further training with additional data. The training data sets appear too small and not representative of the entire range of input parameter values.

One reviewer feels that the discussion of validation in the TBD is lacking. In particular, the reviewer takes issue with the following discussion on page A-29: “The identification of a neural network with the best generalization is better determined with a measure of the test-sample error (residuals of the test or validation data sets), than with the training-sample error (residuals of the training data set).” The reviewer requests clarification as to whether the discussion implies that the test and validation data sets are the same.

3.4 The Overall Quality of the Software and Documentation

- *Comment on the ease-of-use and logic of IWEM.*

All of the reviewers found the EPAIWEM to be user-friendly and intuitive. The reviewers felt that it would be possible to run the software and interpret the results without any documentation. Reviewers felt that the program flow was logical as it led the user from one input to another and that users would need minimal computer and modeling experience to successfully execute this program.

- Comment on the nature of the instructions within the program. Are they clear and easy to understand?

Overall, the reviewers found the software instructions straightforward and easy to work through. The installation was easy and consistent with industry standards. Some of the definition boxes could be expanded, for example, the definition of WMU. In addition, one reviewer felt that it might be useful to have some example justifications for parameters to indicate for archival purposes what degree of information is helpful. Also one reviewer felt that some of the steps within the windows could be more complete. For example, this reviewer wanted more instruction on how to print reports -- the user was frustrated that, when a specific report was selected, that the report did not automatically print.

- *Comment on the layout of the user-interface screens. Are all easy to use and read?*

The reviewers found the user-interface layouts are easy to read and use.

- *Comment on the presentation of results. Are they consistent and easy to understand?*

The reviewers found the presentation of results to be adequate.

- *Comment on the ease of installation and file manipulation (saving and retrieval?)*

Overall, the reviewers found that the program was easily installed and that file saving and retrieval operations were easy to execute. However, one reviewer found that the buttons/icons for reports and printing were lacking in that selecting a report did not automatically result in a print version of the report. The reviewer kept looking around for print or report icons.

- *Comment on the logic and clarity of the documentation. Were any important points, assumptions missing or inadequately explained?*

Overall the reviewers found that the software was so easy to use that the background documentation did not provide much benefit to the user. However, for those users interested in how the tool was developed and trained, the TBD presents significant problems. In many cases, the discussions of the ANN training was inadequate, incomplete, or confusing. See original peer review comments for lengthy, specific comments on the TBD.

- *Comment on the structure of the User's Guide. Is it easy to follow? Are there any inconsistencies with the software?*

The reviewers found that the structure of the User's Guide was well-designed and easy-to-follow. No inconsistencies with the software were observed and/or noted.

- *Comment on the readability of the User's Guide. Can it be used by one without a lot of groundwater modeling experience?*

The User's Guide was praised by all reviewers as extremely easy to use and well-written. In addition, along with the software itself, the reviewers specifically noted that the User's Guide could be easily used by people with very limited groundwater modeling experience.

- *Is there sufficient explanation concerning the training of the ANNs? What aspects of the training should be described? What training parameters and training data need to be presented?*

The reviewers felt that the ANN training methodology is presented in sufficient detail to understand the logic and the process. And that, the aspects of the training discussed are sufficient. However, each reviewer made specific technical comments on areas within the TBD that need to be clarified and/or supplemented.

- *Comment on the readability of the Technical Background Document. Is it written at a level appropriate for someone with some groundwater training and modeling experience?*

The Technical Background Document is easy to read and the logic behind the modeling efforts is easy to follow. The reader level in the document is appropriate with the stated audience.

4.0 CONCLUSIONS

The review panel selected to conduct a peer review of the draft software and supporting documentation for the EPAIWEM, found that the software and supporting documentation were of high technical quality and suitable for use by a wide range of potential users, including those with very limited groundwater modeling experience.

The reviewers, in general, provided significant comments about the discussion found in the TBD on training the neural networks. Reviewers found some of the TBD discussions to be misleading and/or inaccurate, but did not feel that deficiencies in the TBD detracted from the overall quality of the software tool itself.

5.0 REFERENCES CITED

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APPENDIX A

ORIGINAL COMMENTS FROM CURTIS TRAVIS

Review of EPA's Industrial Waste Facility Evaluation Model

By

Stanley Peterson
Thomas McKeon
Curtis Travis
Project Performance Corporation

<u>The Application of EPACMTP to the Tier 1 and Tier 2 Evaluations</u>

General Comments:

The EPA Office of Solid Waste (OSW) has proposed a three tier approach for evaluation of non-hazardous industrial waste facilities. The reviewers of the current documentation have been asked to review the first two tiers of this methodology. Our general observations about the Industrial Waste Facility Evaluation Models and their documentation are as follows:

- We find the two - tiered approach presented by EPA for rapid evaluation of waste management unit designs to be appropriate for the task at hand. It will facilitate evaluation of industrial waste facilities by those with little training in ground water modeling and does not require extensive site-specific data.. The first tier consists of a look-up table based on national characteristics, while the second tier consists on four artificial neural networks (ANNs) trained to simulate the results of EPA's *Composite Model with Transformation Products* (EPACMTP). The second tier allows for a location-adjusted evaluation of industrial waste facilities.

- The use of EPACMTP and its Monte Carlo adaption to compute probabilistic estimates of constituent concentrations in downgradient ground-water wells is appropriate. It allows for estimation of maximum leachate concentrations at the waste facility that will be below MCLs at a monitoring well for 90 percent of the possible cases. Both the EPACMTP and its Monte Carlo adaptation have been extensively reviewed and supported for national level risk evaluations. A probabilistic approach to evaluating maximum leachate concentrations allows for user application with a minimum amount of site-specific data. This allows for rapid and inexpensive screening of industrial waste facilities to determine if more extensive site characterization is necessary. Such an approach will save users time and money and is a definite improvement over a strictly deterministic approach.

- In the Tier 2 analysis, the EPA proposes to use a neural network to approximate the response surface generated by the EPACMTP ground water fate and transport model. The Tier 2 neural network allows for input of site-specific considerations without having to run the EPACMTP model. We highly indorse the concept of using a neural network to approximate the response surface of the EPACMTP model. This is exactly the kind of application for which neural networks should be used.

- The artificial neural network (ANN) training and testing demonstrate ANNs can reasonably predict the general pattern of the EPACMTP model results over a range of input parameters (e.g., see Figures A.3.5 and A.3.12). However, as discussed below, contradictory results and recommendations, problems with the neural network training, and the non-intuitiveness of the input parameters decrease confidence in the code and the ANNs predictive capability.

- The process for selecting the training data set for training the neural network does not appear to be optimal. The current approach is to choose equal frequencies of values over regular increments of input values. This approach gives over emphasis to the tails of the distributions of the input parameters. This has lead to several problems. First, the neural network could not be trained when the total range of the input parameters is used. Thus, input parameter values were restricted to range between the 10^{th} and the 90^{th} percentile. This created the second problem. The neural networks were not trained in a range that contained the infiltration rate assumed for the composite liner (3 x 10-5 m/yr), resulting in unacceptable errors. Thus, the composite liner scenario is not included in the Tier 2 approach for this draft. It is possible that these problems can be alleviated through the use of Latin Hypercube sampling. To be successful, such an approach may require a redefinition of the performance quality criteria so that convergence of the neural network is not overly influenced by the extreme edges of the response surface.

- A major difficulty with the construction of the neural networks in Tier 2 is the choice of the seven parameters used in the prediction of the LCTVs. The seven parameters selected to develop the neural networks were: waste area, infiltration rate, chemical-specific Koc, chemical-specific decay rate, depth to water table, aquifer thickness, and distance to monitoring well. There are two difficulties with this list. First, it would be better to use fewer input parameters in the construction of the neural networks,. The large oscillations of the neural network fits to the EPACMTP results (Figure A.2.3) indicate that there are either too many inputs parameters or too many neurons in the hidden layer of the neural networks. Both of these problems could be fixed with fewer input parameters. Second, this list omits important parameters such as the ground- water flow rate (the product of the aquifer hydraulic conductivity and the hydraulic gradient) which, along with the retardation factor and the distance to the monitoring well, determines the contaminate travel time. The ground-water flow rate is important because it effects both the time the maximum concentration reaches the monitoring well and the time during which contaminate degradation has to occur.

- The ANN predictions have a significant apparent scatter around the baseline model predictions even with the log transformed concentrations of the plots' y-axes. We assume the observed scatter of the ANN results is caused by over prescribing the number of input regression parameters, similar to fitting a higher order polynomial with a typical least squares regression. If this is correct, it may be possible to reduce the observed scatter by combining selected input parameters based on the important physical processes the system is representing. We suggest grouping selected parameters together so that the total number of training parameters is reduced. For example, combining the surface area and infiltration rate defines the mass flux of chemical to groundwater which should be one of the most important parameters in predicting down-gradient concentrations. Another example would be to combine hydraulic conductivity, gradient, Koc and fraction organic carbon. As discussed in the following paragraphs, a further extension of parameter grouping (to reduce the total number of parameters used in the ANN training) would be the use of dimensional analysis to define the minimum number of necessary dimensionless groups and use those dimensionless groups as the ANN training parameters.

- Another important consideration in the choice of optimization algorithms is that neural nets are often ill-conditioned especially when there are many hidden units. Algorithms that use only first-order information, such as steepest descent and standard Back Propagation, are notoriously slow for ill-conditioned problems. Unfortunately, the methods that are better for severe ill-conditioning are the methods that are preferable for a small number of weights, and the methods that are preferable for a large number of weights are not as good at handling severe ill-conditioning. Therefore for networks with many hidden units, it is advisable to try to alleviate ill-conditioning by standardizing input variables and choosing initial values from a reasonable range.

- It should be possible to improve predictability, over the most important range, by limiting the range of DAFs over which the code is trained. For example, for those constituents which have Toxicity Characteristic Regulatory Levels, it is only necessary to accurately compute DAFs up to approximately 100. When the calculated DAF is greater than approximately 100, the LCTV will be capped at the Toxicity Characteristic (TC) Rule Regulatory Level. Accordingly, for constituents covered by TC levels, the ANN could be trained on DAFs ranging from 1 to 100 which would improve the predictability in the range of importance. A similar analysis could be conducted for the rest of the chemical constituents found in the code as the maximum leachate concentration for these constituents is capped at 1,000 mg/l. Therefore, for these constituents it also should be possible to further limit the range of DAFs over which the ANNs are trained.

<u>Response to Questions Raised in the Charge to the Review Panel.</u>

Comment on the tiered approach to analysis of the WMU liner-design. Does it serve the intended purpose?

The tiered approach was designed to accomplish two objectives: (1) allow for the two cases of sites with very little information concerning hydrology and for sites with a much more complete characterization of ground water hydrology, and (2) facilitate modeling by those with little training in ground water modeling. The two-tiered approach presented in the document accomplishes both objectives. The two-tiered approach is reasonable in that it permits users with varying degrees of site characterization data to obtain an immediate analysis and recommendation. Those with little site-specific data can use EPACMTP model results based on national-level data that will result in LCTVs that would be protective anywhere in the nation. Those with more site-specific data can input the data into the appropriate neural network and obtain more site-specific LCTVs.

The look-up table and neural network approximations used in the two-tiered approach permit the EPACMTP ground water code results to be used by a much larger number of users than would be otherwise possible. Thus the objectives of immediate analyses and applicability by a large number of users with differing degrees of existing site hydrogeologic data are met by the two-tier approach.

Given the assumptions for the Tier 1 evaluation, is EPACMTP an appropriate tool to use? Are the results appropriate for the type of analysis?

The EPACMTP is a sate-of-the-art ground water fate and transport computer code that has received extensive peer review by the EPA Science Advisory Board and other review committees. It simulates one-dimensional, vertically downward flow and transport of contaminants in the unsaturated zone as will as two-dimensional or three-dimensional ground-water flow and contaminant transport in the saturated zone. Probability distributions of input parameters were obtained from a nationwide survey of industrial non-hazardous Waste Management Units and their surrounding hydrogeologic characteristics .EPACMTP accounts for chemical and biological transformation processes and is capable of determining overall decay rates from chemical-specific hydrolysis constants using soil and aquifer temperature and ph values. We believe that given the extensive peer review that EPACMTP has undergone and its previous wide-spread application by EPA, the current application of EPACMTP as the basis for EPAIWEM is appropriate.

Is EPACMTP an appropriate tool for generating the response surfaces modeled by the artificial neural networks? Is there another tool or modeling approach that would serve the purpose of the Tier 2, location-adjusted evaluation?

Because EPACMTP is a mechanistic code that is run in Monte Carlo mode, it is an appropriate tool for generating the response surfaces modeled by the artificial neural networks. Running in Monte Carlo mode permits the response surface to be readily generated without manually inputting separate input parameters for each run as is required in a typical mechanistic code.

<u>The Assumptions and Parameters Used to Develop the Tier 1 and Tier 2 Evaluations</u>

Comments on the assumptions and parameter ranges used for developing the Tier 1 national Evaluations. Are the assumptions appropriate for the type of analysis? Are the parameter ranges reasonable?

Tier 1 consists of lookup tables of the maximum leachate concentrations of chemical constituents that, after dilution and attenuation during transport through the ground-water pathway, would not exceed health-based concentrations at a monitoring well 150 m from the waste management unit. These concentrations are derived by modeling with the EPA's ground-water fate and transport model EPACMTP. This approach is straight forward and is appropriate for the current analysis and similar to approaches taken in the past. The EPACMTP model has received extensive review by EPA's Science Advisory Board and has been approved for national-level risk evaluations, such as the current application.

The assumptions and parameter ranges used in Tier 1 appear reasonable. However, we have the following comments regarding these parameters and their associated ranges.

-The time period (10,000 years) during which contaminate migration is modeled seems excessively long. No existing ground water model can produce accurate results over this time period. However, if it is recognized that the Tier 1 and Tier 2 application of EPACMTP is in support national-level risk evaluations and not site-specific ones, this time period may be justified.

-There is some confusion possible with regard to placement of the monitoring well. In Tier 1, the monitoring well is located 150m downgradient on the plume centerline. In Tier 2, the monitoring well is located within plus or minus 90 degrees of the plume centerline and at varying distances downgradient. This distinction is not made clear until page 45. It should be discussed in the section on the conceptual model (page 5) or at least before Table 3-4 an page 35. This table implies that both angle of well off plume centerline and radial distance to downgradient well are stochastic variables. At this point in the document, it has not been mentioned that there is a difference in the way Tier 1 and Tier 2 are evaluated.

-In Table 3-4 it is not mentioned that some of the parameters are on a log scale, while others are not. For example, the median value of WMU area is given as 4.21 square meters. This must be on a log scale.

-The hydrolysis rate (RLAM1) is identified as one of the most sensitive input parameters. No mention of a chemical-specific biodegradation rate is made in the discussion of sensitive parameters. We assume that this is because all transformation reactions are represented by the same first-order decay process and that the hydrolysis rate constant RLAM1 accounts for oxidation, hydrolysis, and biodegradation. It is not clear if any biodegradation rate was assumed in the EPACMTP Tier 1 and Tier 2 calculations. This should be made clear in the text. The median and range of decay rates is not given in the text. Table 3-4 gives the median value for the hydrolysis decay rate and tables 3-5 and 3-6 give decay rates ranging from 0 to 0.1 yr-1. Since this is an important parameter, the document should give the range used to compute tier 1 and tier 2 output.

-It would be nice to know the relative importance of dispersion, dilution, and degradation in the computation of the dilution/attenuation factor (DAF). This information would tell WMU operators if it is worth obtaining site-specific biodegradation data for use in a Tier 3 analysis to improve the calculation of DAFs.

- For the tier 1 analysis, different oxidation states were considered for chromium but not for selenium and arsenic which are also commonly found in varying oxidation states in groundwater. Arsenic and selenium also exhibit different K_d values in different oxidation states. The approach is conservative, however, in that the given oxidation states are generally more mobile.

- Hydrous ferric oxides will tend not to be found in reducing groundwater environments which constitute a large proportion of sites. This method for determining K_d values seems best applied on a site-specific and not on a national tier 1 analysis. Further, we have seen a limited number of sites where hydrous ferric oxide (HFO) data are collected. The range of values (HFO) used for the modeling is most likely hypothetical with little data to support the assumed values.

- The MINTEQA2 approach used assumes that no adsorption occurs when no HFO is present which is incorrect. It would seem more defensible to forget the MINTEQA2 approach (except for site-specific Tier 3 analyses) and use the substantial number of K_d values available for varying soil types to develop empirical relationships (as was done for the Tier 2 analysis). We assume the HFO contents were adjusted to conform to empirical data in any case given the paucity of site HFO data.

- Using a divalent cation, nickel, to represent a monovalent cation, silver, is not conservative.

- The assumption that the leachate pulse duration is the same as the operating unit's life is not conservative. Leachate will continue to migrate from the operating unit after the assumed operating unit's life is over because of continued leaching of waste already applied to the operating unit. The assumption that remaining waste is either removed or has negligible additional contribution to leachate is not conservative and is unrealistic.

Comments on the approach to estimating infiltration for the various WMUs and liner designs. Is the ... long-term liner maintenance?

EPA has chosen to evaluate three types of liner scenarios, the no-liner, single-liner, and the composite-liner scenarios. For the no-liner scenario and the single-liner scenario, EPA used the HELP model to estimate infiltration rates. For the composite-liner scenario, EPA computed infiltration using the liner leakage equation developed by Bonaparte et al.

We assume from Table 3-4 that the infiltration rate is the most sensitive of the input parameters used in EPACMTP. It is therefore important to have good estimates of this parameter. The document should give documentation for the choice of the range of infiltration rates given in Table 4-1, 4-2, and 4-3 for the no-liner and single-liner scenarios. It should also explain the differences for these rates in the tables for landfills, surface impoundments, and Waste Piles. Why is the infiltration rate of 3.1x10-4 m/yr for the surface impoundment composite liner (Table 4-2) less than the infiltration rates for composite liners in Tables 4-1 and 4-3? In contrast, infiltration rates for no liner and single liner in Table 4-2 are larger than the corresponding infiltration rates in Tables 4-1 and 4-3.

The assumption of a single leak per acre for calculation of infiltration rates for composite lines is questionable. In a survey of 28 geomembrane-line units, Darliek (1989) found an average of 10 leaks per acre. Dr. David Daniel of the University of Texas has stated (short course on clay and geomembrane liners, 1991) that the best quality control during liner installation results in approximately one leak per acre while poor quality control results in approximately 30 leaks per acre. An approach that is more consistent with the rest of the modeling would be to sample a range of geomembrane leakage rates using actual data from studies (e.g., Darliek, 1989) as opposed to a single leakage rate. This would be more consistent with the Monte Carlo sampling of a range of values used for other parameters.

The major point to be derived from the “Sensitivity Analysis of Composite Liner Leakage Rates”(Appendix B) is not clear. It is not clear how Rip/Tears are treated in calculating infiltration rates. This needs to be cleared up.

Three soil types were used to estimate infiltration. The three soil types do not encompass the range of soils and associated hydraulic parameters found in nature. The soil textural triangle contains 12 soil textural classes. The three soils types selected encompass seven of the twelve textural classes. Representative particle size distributions for the three soil types provide a high degree of variability in that they encompass a majority of the soils found in the soil textural triangle. The soils chosen, however, and their attendant hydraulic conductivities do not address soils that are essentially sands or clays. Soils classified as loamy sands or sands will have less clay than the coarsest-grained soil used (sandy loam) and will have hydraulic conductivities that may be an order of magnitude or more higher than a representative hydraulic conductivity for a sandy loam. Conversely, the finest-grained soil selected (silty clay loam) will typically have less clay than soils classified as sandy loams, silty clays or clays. The silty clay loam may have a hydraulic conductivity an order of magnitude or more higher than the three soil types mentioned.

Comments on the parameters used for the Tier 2 Location-adjusted Evaluation. Are the parameters appropriate to the type of analysis? Are they parameters that would generally be known about a site? Should more parameters be included? If so, which ones? Should parameters be deleted?

Tier 2 consists of four separate artificial neural networks that have been trained to simulate the results of EPACMTP. The neural networks allow for input of the seven most sensitive site-specific hydrogeologic and waste-unit parameters and output leachate concentration threshold values (LCTVs) . The use of neural networks as an approximation to EPACMTP accomplishes two purposes: (1) it allows estimation of LCTVs by users with no experience in running ground water models, and (2) it is vastly faster than a complete run of the EPACMTP model.

Based on the modeling that was conducted, seven parameters could be used to obtain accurate predictions for each of the four waste types. Using more parameters (12) high correlations were obtained but the results were less predictive than with seven parameters. One anomaly appeared with the reduction of the parameters from 12 to 7. An organic carbon partition coefficient (Koc) was listed as one of the seven parameters but there was no associated organic carbon number. Organic carbon numbers were dropped in moving from 12 to 7 parameters. In a mechanistic sense, one needs an organic carbon number to be able to use a Koc. In a probabilistic sense, the higher Koc values will produce more retardation than lower Koc values.

We pointed out above that we believe the choice of the seven parameters used in the Tier 2 analysis is inappropriate. At minimum, several of the parameters should be combined.

The ANN predictions have a significant apparent scatter around the baseline model predictions even with the log transformed concentrations of the plots' y-axes. We assume the observed scatter of the ANN results is caused by over prescribing the number of input regression parameters, similar to fitting a higher order polynomial with a typical least squares regression. If this is correct, it may be possible to reduce the observed scatter by combining selected input parameters based on the important physical processes the system is representing.

Neural networks can be thought of mappings from an input space to an output space. Thus, loosely speaking, a neural network needs to somehow "monitor", cover or represent every part of its input space in order to know how that part of the space should be mapped. Covering the input space takes resources causing networks with lots of irrelevant inputs to be behave relatively badly. When the dimension of the input space is high, the network uses almost all its resources to represent irrelevant portions of the space.

Unsupervised learning algorithms are typically prone to this problem.

A partial remedy is to pre -process the input in the right way, for example by scaling the components according to their "importance". The current application rightly used this approach. However, even when a network algorithm focuses on the most important portions of the input space, the higher the dimensionality of the input space, the more training data will be needed to find out what is important and what is not.

One possible solution for the IWEM neural network would be to group selected parameters together so that the total number of training parameters is reduced. For example, combining the surface area and infiltration rate defines the mass flux of chemical to groundwater which should be one of the most important parameters in predicting down-gradient concentrations. Another example would be to combine hydraulic conductivity, gradient, Koc and fraction organic carbon. As discussed in the following paragraphs, a further extension of parameter grouping (to reduce the total number of input parameters used in the neural network and to make the parameter actually used more useful) would be the use of dimensional analysis to define the minimum number of necessary dimensionless groups and use those dimensionless groups as the neural network input parameters.

- We are not sure of the ultimate importance of the parameters used in the deterministic sensitivity analysis (page 35 of Technical Background document). However, certain of these parameters appear to be unrealistic. Additionally, there appear to be errors in certain values. Parameters in question are listed below.

- The percent organic carbon and fraction organic carbon do not correlate and one of the values is off by an order of magnitude. The ratio of organic matter to organic carbon varies from soil to soil but generally lies in the range of 1.7 to 2.0. Using the values in Table 3-4 the ratio is 18.6. If the organic matter content is correct, then the fraction organic carbon number is an order of magnitude too low which will decrease the probability that it becomes a sensitive parameter and is carried forward in the modeling methodology.

- The hydraulic conductivity provided as a median value (3.2 m/yr) is very low and is representative of a clay. This hydraulic conductivity would not be considered a median value. Is this partly a reason why the hydraulic conductivity was excluded from the final set of input parameters?

- The "median" Koc value (0.8) appears to be extremely low and will help ensure that Koc is not a sensitive parameter to be carried forward. Hydrophobic organic compounds will invariably tend to have higher Koc values. Following are some representative Koc values for organic compounds often of interest (TCE = 130, PCE = 360, benzene = 80, ethylbenzene = 1,100, naphthalene = 940 and PCBs (general) = 530,000. It is difficult to believe this is a median value.

- The WMU area (4.21 m^2) appears extremely small. Is this a log median value?

- The unsaturated zone thickness (1.17 m) is quite shallow. Given the impacts of a capillary fringe, there would probably be surface water at such sites a good part of the year. Median value?

- The aquifer thickness (1.182 m) is shallow. Such an aquifer in most states would not qualify as a drinking water aquifer. Such a thin aquifer helps determine that the plume is highly dependent on the infiltration rate. Is this really a median value?

- When performing a sensitivity analysis on parameters it seems more appropriate to place the well on the centerline. Movement of the well off the centerline will increase the probability that the contaminant plume misses the well and, thus, makes more parameters insensitive.

- There is no horizontal dispersivity listed. Without a horizontal dispersivity it will be difficult for the contaminant plume to reach a well that is not on the centerline. The plume reaching the well becomes, in this case, highly dependent on the landfill area.

- The distance to the downgradient well appears too large. Some discussion of this issue is needed in the document. Tier 1 uses 150 m as the downgradient distance to the monitoring well. Tier 2 treats downgradient distance to the monitoring well as a stochastic variable with a median value of 427 m.

- The decay rates used in Table 3-5 produce long half lives (from 6.9 years to nondegradable) and reflect consideration of hydrolysis only with no biodegradation. This is a conservative assumption but may not be realistic.

- Page 41 lists 50th percentile areas for the four waste types that range from 405 m^2 to 80,900 m^2. Why was 4.21 m^2 used as a median value in Table 3-4. These waste areas support the contention that the area used in the sensitivity analysis was too small.

-The form of the probability distribution used in the sensitivity analysis (page 33 and Table 3-4) is not mentioned. Since the discussion in the document implies that all that was known about the input parameters were the high, low, an median values, we assume that a triangular distribution was used. Is this the case?

<u>The Quality and Appropriateness of the Artificial Neural Network Tool</u>

Comments on the overall approach to developing the neural networks. Was the program used for training the ANNs appropriate?

Since EPACMTP has been previously sanctioned for such applications, the only difficulties that can arise with the Tier 2 approach come from (1) incorrect design of the neural network, (2) too many input variables in the neural network (3) inappropriate training of the neural network, or (4) too large of an error between the neural network predictions and output of the EPACMTP model. We believe that room for improvement exist in all of these areas.

Size of the Neural Network. A neural network with a single hidden layer and N-1 nodes is theoretically capable of approximating any response surface with N patterns. On the other hand, such a neural network may be very difficult to train. There is no way to tell *a priori* whether or not one or two hidden layers will give the best results. Simple response surfaces can be fit easily with a single hidden layer; more complex surfaces require two hidden layers to obtain good fits. General advice is start small because small networks train faster.

The Tier 2 neural networks were developed using a single hidden layer. The response surface of the EPACMTP model is fairly complex. It is a nonlinear function with response surface spanning several orders of magnitude. Since distributions of the input parameters were not specified in the documentation, it is not clear if the EPACMTP function is defined on a compact set; if not the problem is even more complicated. Thus, it may be that more than one hidden layer is required to approximate this surface with minimal error.

Number of Input Variables. As mentioned above, the curse of dimensionality causes networks with lots of irrelevant input variables to be behave relatively badly. It is very difficult to train a neural network with a large number of related input variables. Much of the internal memory of the neural network is taken up learning redundant information. General advice is to use the smallest number of input variables as possible. This will speed up training and decrease the prediction error.

The Tier 2 neural networks have too many input variables. We have pointed out above several ways that this problem can be corrected.

Training the neural Network. Both Back Error Propagation and the conjugate gradient method were used to train the neural networks. Back propagation is a first order method which presumably would be used for initial training, while the conjugate gradient method is a second order method which is more computational intensive and presumably would be used . Page 55, Paragraph 3 implies that only conjugate gradient was used in training. Documentation needs to be clearer on what combination of training was used to train the Tier 2 neural networks, Standard Back Propagation is a euphemism for the generalized delta rule and is the most widely used supervised training method for neural nets. Back Propagation can be used for incremental training (in which the weights are updated after processing each case) but it does not converge to a stationary point of the error surface. To obtain convergence, the learning rate must be slowly reduced. This methodology is called "stochastic approximation." However, the process can be tedious. Too low a learning rate makes the network learn very slowly. Too high a learning rate makes the weights and error function diverge, so there is no learning at all. If the error function has many local and global optima, as is probably the case for the Tier 2 neural networks, the optimal learning rate often changes dramatically during the training process. Page A-15 states that the leaning rates for the Tier 2 neural networks were not modified during training. Training a neural network using a constant learning rate is usually a tedious process requiring much trial and error.

Two methods that are effective at speeding up Back Propagation are Quickprop and RPROP. Concise descriptions of these algorithms are given by Reed and Marks (1999), *Neural Smithing: Supervised Learning in Feedforward Artificial Neural Networks, Cambridge, MA: The MIT Press.* However, conventional nonlinear optimization methods are usually faster and more reliable.

Error Between Predictions and Response Surface. The neural network predictions have a significant apparent scatter around the baseline model predictions even with the log transformed concentrations of the plots' y-axes. We assume the observed scatter of the neural network results is caused by over prescribing the number of input regression parameters, similar to fitting a higher order polynomial with a typical least squares regression. If this is correct, it may be possible to reduce the observed scatter by combining selected input parameters based on the important physical processes the system is representing.

The following are specific comments regarding various aspects of the neural networks:

Page 12, Paragraph 4 states that neural networks can become "over-fitted". This is a neural network that produces excellent results with the training input data, but performs poorly with data it has not seen before. The document states that this problem can be avoided by careful choice of neural network size and the amount of training applied to the neural network. This statement is incorrect. These variables have little to do with preventing the network from becoming "over-fitted". The only way to increase the chance of predicting data that the neural network has not seen is the have training sets that are representative of the total range of model output. A neural network can only predict well those model outcomes that it has been trained to predict. If representations of these outcomes are not in the training set, controlling the network size and amount of training will not improve the neural network performance on data it has not seen.

Page 15, Paragraph 4 states that in training the neural networks, problems were encountered when the extremes of the input parameter distributions were used as input to the training. “Initial attempts to train on data sets that included the full 0^{th} percentile to100th percentile input parameter ranges were unsuccessful” (Page A-4, Paragraph 2). Therefore, to produce the best possible predictive tool with broad applicability and acceptable accuracy, the decision was made to generally train and validate the neural networks using input values in the range of 10^{th} to the 90^{th} percentile. This is a serious problem with the training protocol for the neural networks.

The EPACMTP model results are highly sensitive to the location of the ground-water well. In the Tier 2 analysis, both the radial downstream distance and the angle off-center of the observation well are stochastic variables. This leads to situations where the lateral edge of the plume may not reach to observation well. Thus the observation well would show a zero concentration and lead to the calculation of an infinite value for the dilution/attenuation factor (DAF). There is nothing wrong with this situation, but it is just something to keep in mind. On page 5, the document states that there is a one-to-one correspondence between DAF and monitoring well concentration. This is only true in the deterministic case. In the Monte Carlo case discussed above (where both radial distance and off-center angle of the well vary), multiple locations of the monitoring well can lead to the same calculated value of the DAF. In fact there will be an infinite number of well locations with the same DAF. Again, this is not a problem because in the Monte Carlo case, one uses the 90^{th} percentile DAF as the measure of the amount of dilution and attenuation that would likely occur. However, these points could be clearer in the text.

The selection of a 90^{th} percentile DAF (for DAFs ranked from highest to lowest) as the measure of dilution and attenuation is a policy decision. However, we note that the choice of the 90^{th} percentile is consistent with numerous other EPA analysis including the proposed 1995 hazardous Waste Identification Rule (HWIR). This choice would be protective in at least 90% of possible well locations (within the bounds set for well locations) and therefore satisfies the EPA goal of being protective of the majority of the population.

A serious omission in the documentation of the neural network development is how the necessary one-to one correspondence between neural network input parameters and the EPACMTP model output was established. EPACMTP (run in Monte Carlo Mode) starts with probability distributions for each input parameter and generates a probability distribution for some desired output parameter, in this case the DAF. The 90^{th} percentile DAF was selected as the appropriate measure of dilution and attenuation. Thus the EPACMTP run in Monte Carlo mode sets up a one-to-one correspondence between the probability distributions of its input parameters and the 90^{th} percentile DAF. The purpose of the neural network is to set up a one-to-one correspondence between its deterministic input parameters and the 90^{th} percentile DAF computed by EPACMTP. The document is not clear on how this correspondence is established.

On page 13 the documentation states the trained neural network was used to predict the EPACMTP output value (the DAF) as a function of combinations of EPACMTP input values. This implies that the output of the neural network was a target DAF value. This statement is also made on page 12, paragraph 3. Figure 2-3 also implies that DAF values are the computed output of the EPACMTP model. However, on page A-7 of Appendix A, the document states that the neural networks were trained to predict:

- the peak well concentration (log pk conc) and
- the maximum 30-year average well concentration (log avg conc).

It is important that the document be clear as to the output parameter(s) used to train the neural networks.

Page A-7 of Appendix A states that the peak will concentration was used to calculate the Leachate Concentration Threshold Value (LCTV) for non-carcinogens and the maximum 30-yr average concentration was used to develop LCTVs for carcinogens. Page 5 and 6 state that the DAF is used to compute the LCTV. However, it not mention the relationship between monitoring well concentrations and time. This needs to be made clear.

DAFs are computed using the peak well concentration or the maximum 30-yr average well concentration. Thus, in the Monte Carlo case, DAFs for different wells are computed based on different travel times. This is ok.

We are not sure why it is necessary to compute and list DAFs ranging up to 10^6. For those constituents which have Toxicity Characteristic Regulatory Levels (Table 4.4), generally, it is only necessary to accurately compute DAFs up to approximately 100. When the calculated DAF is greater than approximately 100, the LCTV will be capped at the Toxicity Characteristic (TC) Rule Regulatory Level. Accordingly, for constituents covered by TC levels, the ANN could be trained on DAFs ranging from 1 to 100 which would improve the predictability in the range of importance. For these 39 constituents (Table 4.4) , it does not matter if the DAF is 10^3, 10^4, 10^5, or 10^6; once the DAF is greater than 10^2 the result (LCTV) is the same. A similar analysis could be conducted for the rest of the chemical constituents found in the code as the maximum leachate concentration for these constituents is capped at 1,000 mg/l. Therefore, for these constituents it also should be possible to narrow the range of DAFs over which the ANNs are trained. Again, narrowing the range over which the code is trained will improve the accuracy of the ANNs in the area of importance.

Comments on the number of parameters, the range of values, and the combinations used for training. Is there a training method or approach that would enable inclusion of parameter values spanning many orders of magnitude?

The text states that twelve parameters were selected to develop the neural network but 13 parameters are listed in Table 3-7.

Dimensional analysis of the geometric, flow, and chemical parameters that govern the model prediction of the DAF may be a useful tool to augment or enhance the training data sets for the ANN. The Buckingham Pi Theorem states that any physical relationship can be expressed in terms of independent, dimensionless products composed of the pertinent physical parameters. Using dimensional analysis, the general form of relationships between the quantities can be established and experimentation (i.e., model simulations in this case) is then required to derive the specific coefficients relating the parameters. Dimensional analysis differs from other types of analysis (such as the current model simulations used) in that it is not based on the fundamental principles of mass, energy and momentum conservation. Dimensional analysis is instead based solely on the relationships that *must* exist between the pertinent variables because of their dimensions. Dimensionless parameters (derived from dimensional analysis) are widely used for a broad range engineering design applications including a number of groundwater hydrology and mass transfer applications. In terms of the application to a training data set for the ANN, the appropriate dimensionless parameters may be used to reduce the number of independent parameters, as well as the parameter ranges that need to be included in the training data set. In a sense, the dimensionless parameters are allowing the ANNs to start from a very "intelligent" baseline when defining the most important parameters and corresponding relationships that affect the model-predicted DAFs.

Typical state regulations require a groundwater resource protection standard along with protection of existing supply wells. Based on this implementation of regulations, it may be more appropriate to use a training data set for the ANNs which places the well directly in the centerline of the plume. This may make the final IWEM results more compatible with typical regulatory decision processes. In addition it may provide a training data set which covers fewer orders of magnitude and allows the ANNs to achieve a better fit to the response surface.

The selection of parameters for developing the ANNs initially started with the following parameters: waste area, infiltration rate, Koc, decay rate, product of percent organic matter (unsaturated zone) times the fraction organic carbon in the saturated zone, product of conductivity and gradient (the Darcy velocity), depth to water table, aquifer thickness, angle of monitoring well off the centerline of plume and distance to the monitoring well. Based on initial testing and evaluation of the optimum number of parameters to train the ANNs (presumably based on the degrees of freedom required to match the response surface), a total of seven of the above parameters were selected to train the ANNs. Two of the parameters deleted, the Darcy velocity and the angle of monitoring well off the centerline of plume, would seem to be very important to the ANNs predictive ability. Because the chemical-specific decay rate is included as a parameter, the Darcy velocity which defines the time over which degradation would occur would appear to be very important. The velocity is also used with the dispersivity to calculate the dispersion coefficient in the transport equations (this parameter controls the spread of the Gaussian distribution) and is expected to be important One possibility would be to use the retarded Darcy velocity as a training parameter. This would effectively include the conductivity, gradient, Koc and Fraction organic carbon as a single training parameter. Another possibility would be to include a dimensionless parameter based on the velocity, travel distance and decay rate as a training parameter (possibly including the retarded velocity). As noted previously, it may be appropriate to develop the training data sets using cases where the well is located on the centerline of the plume. If not, it is expected that the angle to the well location is an important parameter unless the waste areas are so large that locations at 45 degree angles from the centerline are still within the bulk of the plume. Intuitively, one would expect that the angle to the receptor well may be more important than other parameters included such as the aquifer thickness or the depth to the water table.

Comments on the quality of the ANNs as described by the various criteria used. Are there other criteria that should be used to evaluate the quality of the ANNs? Is the error between EPACMTP and the ANNs acceptable in the context of the uncertainties associated with groundwater modeling?

The criteria used, such as R^2 values, plot, histograms, etc. were appropriate. Based on the limited result summaries seen, the quality of the ANNs appears good. We question how the data transformations have effected the evaluation of the ANNs effectiveness using the criteria. For example, the coefficient of determination, R^2, will be increased by using log-transformed data. It is unclear whether the predicted and measured concentrations would have exhibited a R^2 that met the stated acceptance criteria (R^2 of 0.9) without manipulating (transforming) the data.

The term “coefficient of determination” is used in the text without prior definition, for example on Page 59, paragraph 4. The definition is given on Page A-19, but appears incorrect and terms are not defined.

Running the code produced contradictory results and recommendations. For example, in certain situations the Tier 2 analysis resulted in higher DAFs for the No Liner scenario than for the Single Liner situation. Because of this, depending on initial leachate concentrations, a chemical would be protective without a liner and not be protective with a liner. In other words, a higher LCTV was achieved under the No Liner than with the Single Liner Scenario. These results contradict reality and diminish confidence in code’s predictability.

Comments on the various approaches used to filling in the response surface for the purpose of getting a better fit between EPACMTP and the ANNs. Is there a method for better incorporating the extremes of the parameter distributions?

One of the biggest limitations of the code is the assumption of homogeneity. Typically, aquifer materials are deposited in stratified layers. Because of aquifer stratification (non-homogeneity), many contaminated aquifers have strongly stratified plumes (i.e. the plume extends over a discrete interval of the aquifer thickness). Currently the model training data sets use a 90th percentile of the aquifer thickness in the range 80 to 90 meters. Although there are certainly a number of aquifers which are this thick, most aquifers have stratigraphic layers which effectively confine the contaminant plume intervals to layers which are on the order of 3 to 10 meters thick. This observed plume distribution is presumably the result of aquifer heterogeneity which typically is not represented in most groundwater modeling applications. In order for the DAF factors to be conservative it may be prudent to consider limiting the aquifer thickness to a typical range of plume thicknesses that have been observed in many cases (i.e., artificially force the model results to limit the plume thickness by constraining the aquifer thickness).

Comments on the approaches to selecting the training, test, and validation data sets.

The process for selecting the training data set for training the neural network does not appear to be optimal. The current approach is to choose equal frequencies of values over regular increments of input values (Page A-9, Paragraph 2). This follows the advice of Swingler (1996) that a training data set should contain a similar number of samples from different “classes” of data that the neural network should learn. However, in training a neural network over the range of the distributions of the input parameters such a procedure will result in an over representation of infrequent values. It would seen more reasonable to use a Latin Hypercube procedure, which selects samples relative to their frequencies, to sample the input parameter distributions to construct the training data set.

The histograms of input values used in training (Figures A.2.6 and A.2.7) do not appear to show equal frequencies for each value over the range of values. There seems to be too much emphasis on using the pure “star-point” distributions. If the “after training” matrix in Figure A.2.6 is any indication, the training set used for LOGAREA was nowhere near uniform. As the sensitivity analysis pointed out, LOGAREA is one of the most important parameters. With so little of the training space used in training, one wonders if training can be efficient. If obtaining equal frequencies fir the training input values is deemed important, we would suggest choosing the training input values by sampling randomly from a uniform distribution of the range of input values. We believe that this is an important point since a neural network can not learn to predict a portion of the response surface that it has not been trained on.

In general, it appears that the neural network predictive capability would be improved through further training with additional data. The training data sets appear too small and not representative of the entire range of input parameter values.

The modeling tool used state-of-the-art methodologies to emulate the output from the

EPACMPT code. The tools it used in conjunction with the methodology appeared to be well thought out and appropriate. The intended purpose was met in that a high degrees of correlation was obtained between the EPACMPT outputs and the predictions made by the IWEM model.

<u>*The Overall Quality of the Software and Documentation*</u>

Comments on the ease-of-use and logic of IWEM.

The documentation is more than sufficient. The program is user friendly and intuitive. It would be possible to run IWEM and interpret the results without any documentation.

Comments on the nature of the instructions within the program. Are they clear and easy to understand?

Very user-friendly program. We ran the program without reading the documentation and it was easy to follow. The program flow was logical as it lead you from one input to another. A user would need minimal computer and modeling experience to successfully execute this program.

Comments on the layout of the user-interface screens. Are all easy to use and read?

The user-interface layouts are easy to read and use.

Comments on the presentations of results. Are they consistent and easy to understand?

Comments on the ease of installation and file manipulation (saving and retrieval?)

The program was easily installed. The file saving and retrieval operations were easy to execute.

Comments on the logic and clarity of the documentation. Were any important points, assumptions missing or inadequately explained?

The documentation is easy to follow. Given the ease of use of the program, the documentation provides little benefit.

Comments on the structure of the user's guide. Is it easy to follow? Are there any inconsistencies with the software?

The User's Guide is easy to follow.

Comments on the readability of the user's guide. Can it be used by one without a lot of groundwater modeling experience?

> The User's Guide is readily understood and could be used by one without previous groundwater modeling experience.

Comments on the structure of the Technical Background Document. Is the modeling approach and logic used for development of the ANNs clear?

> The modeling approach and logic used for development of the ANNs is clearly presented in the Technical Background Document.

Is there sufficient explanation concerning the training of the ANNs? What aspects of the training should be described? What training parameters and training data need to be presented?

> The ANN training methodology is presented in sufficient detail to understand the logic and the process.

Comments on the readability of the Technical Background Document. Is it written at a level appropriate for someone with some groundwater training and modeling experience?

> The Technical Background Document is easy to read and the logic behind the modeling efforts is easy to follow.

Typographical errors: We never looked for typographical or grammatical errors but noted the following errors in the documentation.

TECHNICAL BACKGROUND DOCUMENT:

Page 45, second line; should be while not wile

Page 57, second line; should be " ... data it had not..." not as written "....data is had not..."

Page A-40, last line, second paragraph; should be ...values are high *and* concentrations are low.

APPENDIX B

ORIGINAL COMMENTS FROM DONNA RIZZO

4) Methodologies and Assumptions used in the Groundwater Pathway Modeling

Overall, this is a very good first-generation groundwater pathway model. I believe the work presented to be thorough and accurate. My major concerns lie with the *written portion* of the Technical Background Document (TBD) – specifically the presentation of the Tier 2 neural network model. Although, I believe the IWEM software and the underlying models to be of high quality and technically sound, the overall organization, and re-definition of standard artificial neural network (ANN) terminology in the TBD, detract from the understanding and the credibility of the underlying models. Two overall suggestions for a second-generation Tier 2 ANN model follow. More specific revisions to improve the quality and understanding of the TBD, and as a result, the underlying Tier 2 ANN model may be found in item 3 below.

The authors should provide some justification for selecting the method of backpropagation (specifically NNModel version 3.2). On page 53, (third paragraph, first sentence) the authors state,

> ***"Therefore, the first step in developing neural networks to approximate EPACMTP was to determine an appropriate set of EPACMTP input parameters that would be used to predict the outcome of EPACMTP, the concentration of a chemical in a downgradient ground-water well used for drinking water and its inverse the DAF."***

The *first step* should be the selection of an ANN (computational tool) to address the task at hand. Although the developers have selected the method of backpropagation to address the problem of approximating the EPACMTP, other algorithms exist that might have been more appropriate for this particular task. Backpropagation is a gradient descent method that notoriously requires long training times and is prone to converging to local minima instead of finding the global minimum error surface. All training algorithms that make weight adjustments to continuously reduce the objective function are prone to this problem of local entrapment. Although backpropagation is the only ANN algorithm provided by Neural Fusion (1998), other algorithms exist that would have greatly simplified the lives of the developers. If one of the goals was to find an algorithm that would approximate processes in the same manner as regression analysis, then the developers may want to consider the General Regression Neural Network (GRNN) in a second-generation model. The GRNN algorithm has its theoretical foundations in regression analysis and requires very little training time.

If the developers choose to remain with backpropagation, one additional suggestion for a second-generation model is to implement modular ANNs (*i.e.* have separate ANNs for ranges of data where the training patterns appear to compete with each other). For example, since the significance and sensitivity of the input parameters change greatly for MWUs with low monitoring well concentrations and high monitoring well concentrations (or alternately low and high infiltration rates), separate ANNs might be considered for these two regions. This would not only help the predictive capability of the

backpropagation networks but it would greatly reduce training times.

In addition, at the bottom of page A-29, the authors state,

"In general, the neural network predictions for input parameters outside the 10'th to 90th percentile values will likely be less accurate than for input values within this range."

This is true. In fact, the neural network should not really be used to predict values in a range that it has not been trained on. When running the model, the user is warned that he/she is outside the input parameter range and asked if they would like to proceed. This is a nice feature of the IWEM graphical user interface. However, if it necessary for the ANN to make predictions outside the 10th to 90th percentile range, then a second-generation model should include separate ANNs that are trained on data in each of these ranges (0th to 10th and 90th to 100th).

Performing principle component analysis of the data prior to selecting the subset of input parameters would also be advantageous. This would help justify why the backpropagation network did not perform well, when all 10-12 input parameters were considered, and identify additional regions of the input parameter space in which to modularize the ANNs (create separate ANNs).

Despite the hardships encountered when training backpropagation algorithms, I believe the selected algorithm to be appropriate for the problem at hand and the end product (given the size of the problem that was undertaken) to be commendable. As stated above, my greatest concern lies with the manner in which the TBD is organized and the *written description* of the Tier 2 model and its training procedure. Confusion exists throughout the document with regard to definitions and terminology used to describe the Tier 2 ANN. Specific recommendations are provided in item 3 below.

5) Utility of the Software

The IWEM software package is very intuitive and the graphical interface is extremely user friendly. In my opinion, most users will be able to install and run the software without reading the IWEM Users' Guide.

The IWEM Users' Guide is both concise and well written. In fact, reading the introduction (section1) of the IWEM Users' Guide prior to reading the TBD, would have greatly improved the overall flow and understanding of the TBD. With the exception of one remark (below), all comments and suggestions regarding this Guide and software are minor and can be found in the margins of the hard copy.

On page 5 of the IWEM Users' Guide the authors state,

> ***"Therefore, where appropriate in Tier 1 and Tier 2, EPA used ranges of parameter values that result in a high estimate of risk to ensure the protection of groundwater."***

Is this high estimate of risk a result of selecting a *wide* range of parameter values or the result of a *conservative* range of parameter values?

(Note: I do not feel qualified to judge whether the ranges of values provided in the IWEM Model (also in Tables 4.2-4.5) are sufficiently large to accommodate most existing and proposed WMUs.)

6) Recommended Approaches for Revision and Improvements of the " Technical Background Document: Industrial Waste Management Evaluation model (IWEM), Ground Water Model to Support the Guide for Industrial Waste Management"

I. Recommendations Re: Improving the Overall Flow of the TBD:

1. The two-tiered approach (currently described on page 17 in section 3.0) should be presented before section 2.3 – Development of Neural Networks to Emulate Ground-Water Models (see pages 9-16). Currently, details of the Tier 2 ANN used to simulate the results of the EPACMTP (including specific input and output parameters) are described before the user has been introduced to the two-tiered approach.

2. A very nice introduction and description of the four different waste management units (WMUs) of concern: landfills, surface impoundments, waste piles, and land application units, is presented on page 1 of Appendix A. This should be done much earlier in the document (*i.e.* prior to the description of no-liner, single clay liner, and composite liner).

3. (p. 22-28) The *general* description of the four graphs used to document the ANN training process using *specific* data, is difficult to follow. This section needs to be re-written.

4. The text at the bottom of page 64 and the top of page 65 explains that the Tier 1 National Evaluation does not require site-specific data and that the ANN approach includes a Location-Adjusted Evaluation. The specific goals of each Tier should be introduced prior to this description.

5. The write-up of sections 3.2 and 3.3 appear to have gone through much more review and revision. These sections are nicely written and the model assumptions are clearly

defined. Moving this material earlier in the document would greatly help the flow. Perhaps repeating the first 7 pages of the IWEM Users' Guide at the beginning of the TBD would help the overall organization of the document.

6. (page A-7, first paragraph, last two sentences)

> ***"Modeling the landfill scenario with EPACMTP assumes an essentially steady-state scenario in which the organic carbon partition coefficient (KOC) has little or no effect on the output. Therefore, the landfill neural network did not consider KOC as an input parameter and did not use the average peak 30-year concentration as an output parameter."***

The latter part of this last sentence (in bold above) does not logically follow from anything stated in the previous sentence (or paragraph). How does a steady-state scenario with KOC having little or no effect on the output, justify the elimination of one of the ANN output parameters (max 30-yr ave. well conc.)? Was this output parameter eliminated due to complications in training? This explanation needs to be clarified. (Note: Comments are being addressed in chronological order. There are two or three places near the end of the Appendix in which statements (that appear illogical earlier in the document) are addressed. For example, the justification for choosing only one output parameter for the landfill neural network is clarified in the first paragraph of subsection A.3.1.1 on page A-32. This should be stated much earlier in the document. Other places where similar confusion occurs are noted below.

II. Recommendations Re: ANN Terminology – specifically focussed on Training and Validation

Training

1. The authors appear to be confusing the terms "training" data sets, "test" data sets, and "validation" data sets throughout the TBD. Near the bottom of p. A-19, the authors state,

> ***"The goal for each neural network was to reach an R2 -value greater than or equal to 0.9 for both the training data set and the test/validation set."***

Does this imply that the "test" and "validation" data sets are the same? If so, this appears to contradict earlier discussions of these two data sets (see for example, the description and labels "training/testing" and "validation" used in Table 5-1). Also, the

$R2$ value associated with surface impoundments is 0.825 – this is not greater than the value 0.9 presented on this same page.

Item 4 on the bottom of this same page states, "the $R2$ -value for the training and validation set decreased". It is not possible for both of these $R2$ values to decrease simultaneously. Once training has been performed and an acceptable $R2$ value has been achieved, the ANN weights are fixed before validation begins. This is the traditional definition of a validation data set.

2. (page A-2) The $R2$ value during training should reflect the true value obtained for *all* the training patterns - not a "test data set of *predetermined* input parameter combinations" used to optimize the generalization capability of the ANN. The traditional use of the term "test data set" or "validation data set" is a set of data used simply for the purpose of testing the predictive capability of the trained ANN.

Although the Neural Fusion (1998) NNModel does have a slightly different definition for "test data set", this definition is not common knowledge. As I understand it, these strategically predetermined data points were generated to improve the generalization capabilities of the training data set. In general, this is simply a part of the process necessary to generate a training set that 1) has an adequate number of data points, and 2) adequately spans the range of data values being used for prediction. On page A-8 the authors state,

> ***"Based on the results of testing the neural networks, in some cases test data were transferred into the training data sets."***

This is what should be done to create a training set. The training set should be *ideally* generated (balanced, general, accurate, *etc*.). The authors should omit references to "initial" training set and simply describe the training set used to produce the results of this investigation. If what the authors are calling a "test" data set and "validation" data set are later used to "train" the ANN (*i.e.* fix the internal weights before using the network for prediction purposes) they should not be referred to as "test" and "validation" data sets! They are then part of the "training" set (and should be a part of the data used to obtain the $R2$ value for training).

In my opinion the authors should remove all references to the phrase "test" data (when referring to data that was later incorporated into the training data set), and use the word "validation" or "test" to refer to the separate unbiased data used to test the trained ANN. There are well-documented ways to generate test cases. The method(s) used for identifying good "training sets" for this investigation should be discussed in the Appendix.

However, if the authors choose to use Neural Fusion's definition of "test" data set, a description of the type provided on the bottom of page A-32,

> ***"The landfill neural network consisted of a training data set and a test data set, a second training data set to cover more data space in the input variable space, and finally, a validation data set to evaluate the performance of the final neural network."***

placed earlier in the document is mandatory. It will greatly reduce some of the confusion between "training", "test", and "validation" data sets. It is not until page 56 of Appendix A that the authors finally state that the initial training and test data were combined into one data set. It is important to explicitly state this earlier in the document. However, even at this stage in the document, the reader is never told which of these "training/test/validation" data sets were used to train the neural networks used in the IWEM (*i.e.* used to fix the weights of the ANNs before they are used for validation and/or predictions). If additional "test" data sets are used in training the weights of these ANNs, then these "test" data sets should not, in my opinion, be called "test" or "validation" data sets. As far as the end user is concerned, they are part of the "training" set and have been used to adjust the internal weights of the final ANN used for prediction purposes.

3. (page A-8, second paragraph) In describing the derivation and range of the test data set,
I believe the authors are again confusing "test" data sets with what they call "validation" data sets earlier in the document (see page A-2 and the overview of Neural Network Training and Testing Process Figure A.2.1).

4. (pages A-51 and A-52) Figures A.3.9 and A.3.10 are identical for final and test data sets.
Is this accurate?

5. The 95% confidence interval graphs for the training and test data sets (pages A-78 and A-79) are identical (including the slope and intercept of the regression lines to four decimal places). If this is the case, then the test data set is not a valid test data set and should not be labeled as such.

Validation

1. (page A-29, first paragraph, last sentence)

"The identification of a neural network with the best generalization is better determined with a measure of the test-sample error (residuals of the test or validation data sets), than with the training-sample error

(residuals of the training data set)."

Are the authors now implying that the test and validation data sets are the same? Or are they implying that there are three measures of error (training, testing and validation)? If the latter is true, then the R^2 values for all three data sets should be shown somewhere in this document. (Note: only two have been shown in Table 5-1 on p. 26 – the R^2 value for the training data set and the R^2 value for the validation data set.)

2. (p. A-35)

> ***"The landfill neural network, the first neural network developed out of the four, was not integrated with an additional fully random validation data set."***

Again, by definition, "validation" data sets should be an independent, unbiased set of random data points and should not be integrated into the "trained" neural network. The hidden weights of the neural network should be adjusted during training and fixed prior to validating the ANN model. If the developers want to integrate these "validation" tests into the end product (four trained neural networks) this is fine, however, it should not be described in this manner (part of the testing and validation) in this document.

In addition, in the above statement, the authors refer to the validation data sets as fully random and in other places of the document as sequentially random and essentially random. These adjectives do not instill confidence in the reader that the data sets are indeed random. If they are random, remove the adjectives. If they are not random, explain why.

3. (page A-59) If the 1144 validation data examples were appended to the training matrix (*i.e.* used to train the internal weights of the final ANN) they should not be referred to as "validation data examples".

Other Recommendations

1. Several of the definitions contained in the glossary are not accurate. For example, the sentences used to define the backpropagation method are not sufficient. These statements are true of many ANNs and do not provide the reader with a definition of backpropagation. Many of the other definitions are too general; while others are specific only to the method of backpropagation (see additional remarks in the hard copy).

Also, the document should contain a statement somewhere (in the introduction?) indicating that a Glossary exists.

2. (page 10, last paragraph) Given the very general nature of the overview provided for ANNs, the authors should probably delete the sentence -

"The hidden node values are analogous to regression equation terms and weights are analogous to the coefficients in a regression equation".

Although the attempt to "de-mystify" ANNs and discuss the analogy between many of the connectionist ANNs and classical regression analysis is admirable, for readers with experience in the field of ANNs, this sentence will instill skepticism. This sentence is true of many ANN algorithms, but the theoretical foundation for each algorithm differs. In addition, the particular algorithm selected in this study is Backpropagation (Note: the reader does not know this until page 55, section 5.2). In general, backpropagation is a gradient decent method, and although under certain assumptions and constraints it is analogous to classical regression analysis, there are many other ANNs with theoretical foundations more rooted in these classical regression techniques.

3. (page 12, first sentence) The authors are confusing ANN "architectures" with "types" of ANNs. The multi-layer architecture depicted in Figure 2-4 is simply that – a multi-layer "architecture" (as opposed to a single-layer architecture). The reference to radial basis functions and self-organizing maps is out of place in this paragraph. Both of these "types" of ANNs are capable of having the same multi-layer architecture depicted in Figure 2-4. It is true, as the authors state in the second to last sentence of this paragraph, that the MLP is the most successful and widely used neural computing tool. However, the web site http://www.spss.com cited by the authors is referring to *architecture* and not *types* of ANNs.

4. (top of p.59) The authors are confusing the terms "data sets" with "data points" (traditionally known as data patterns or data vectors). I believe that line 1 of Table 5-1 (mislabeled Table 5-7 in text) which currently reads,

"Number of training/testing data sets",* should read *"Number of training/testing points (or patterns)"

where a training point (or pattern) is defined as the vector (single row of the matrix described on p.57 and shown in Figure 5-2) containing both training input parameters (log KOC, log area, SINFIL, DSOIL, ZB, log radius) and the corresponding output parameters (log ave. conc., and log peak conc.) predicted using EPACMTP. The number of data points used for training and testing should be indicated in this Table.

However, if the authors really intend for this line to read "training/testing sets" then the

number of points or patterns used in each set should be defined to provide the user with some degree of confidence in the size or breadth of the training sets.

In addition, I believe the line identified as "Number of validation data sets" should read "Number of validation data points" where a data point should be defined as one set (row vector) of inputs and corresponding outputs spanning the training data space.

5. (page 63) The authors are confusing the $R2$ values for training and validation. The value should read 0.825 and not 0.992.

6. (page A-14) The second bullet reads-

"Maximum number of hidden neurons and hidden layer addition".

Should the "hidden layer addition" read "the addition of hidden layers"? The same confusion between layers and neurons exists on p. A-17 (middle of the page, first bullet) "Hidden layer addition: Fixed # of hidden neurons". My understanding is that the four ANNs developed in this work used *one* hidden layer and a different *fixed* number of hidden neurons for each of the four networks. Is this assumption accurate?

7. (Figure A.3.4, page A-39) The test data should span (be balanced over) the entire range of values used for training the network. The measured and predicted DAF values (see Figure A.3.4) are clustered in the ranges between 0 and 1 and around 3. Is there a reason for this? How does the user know that the $R2$ values are not 'selectively" high? Are the $R2$ values lower for test data that are more representative of the entire range of data values?

Also, the 95% confidence interval graph (PI-Graph) is the most informative/useful of the tools shown in this document for purposes of evaluating the neural networks. Why are these graphs not shown for the validation tests of each network?

8. (p. A-45) Item 5 and the last paragraph on page A-45 summarize everything that was stated in the previous two pages. The authors are making the discussion of "selecting training data" much more complicated than it has to be. These two pages could be condensed into one or two paragraphs. (All references to "tallest and shortest neighboring columns" and "no columns" should be removed and replaced with references to " where the frequency distributions are high", "low", or where "data does not exist".)

9. (pages A-54 and A-55) Why show only partial validation results in tabular form? Why

not use the same 95% Confidence Interval Graphs that were used for testing and show all of the validation data?

10. (page A-17, middle of the page, second bullet) "Stop network on criteria: None" Does this bullet imply that the network convergence is based solely on the maximum number of iterations (or what the authors refer to as "total counts") and not some tolerance criteria such as a root-mean-square error value? If yes, this is important and should be explicitly stated.

11. (page A-23) The authors discuss the tolerance (acceptable error of the total error) being used as a criteria to end the training process, however, the authors also state in the last sentence of this same paragraph;

> ***"The tolerance can generally be used as a training stopping point. However, this option was not applied to the development the four neural networks."***

Why? What is the acceptable error used in this work, and the tolerance level at the end of each training process?

12. (page A-40)

> ***"Interrogation of the landfill neural network.......showed the neural networks ability to predict output values close to the desired EPACMTP output values for most of the data samples, especially for low range DAF values (1-1000)."***

This statement doesn't appear to correspond to the results of Figure A.3.5 on page 40(?).

14. (page A-43, Table A.3.4) Why are there two columns in Table A.3.4 entitled "CMTP runs" and "RUNS used"? Does this imply that all of the "runs" were not used? If so, why not?

III. Other Recommendations:

1. Explicitly state that soil type and geographic location are considered when using the IWEM software. If one reads this document prior to running the software, the connection between infiltration rates and soil properties is not clear.

2. (page 15) In the first paragraph of section 2.5, are the location-specific data different than the input parameters used (and/or listed on p.13) to train the ANN? The use of the

term *location-specific* data and *site-specific* data should be defined (and why not use the same term throughout the document?). In addition, the sentence in the second paragraph –

> ***"Thus, the Location-Adjusted Evaluation allows the user to instantaneously evaluate a number of site-specific considerations without having to run EPACMTP or another ground-water fate and transport model"***

is confusing. The reader is assuming at this early stage in the document that the ANN output consists of a single DAF estimate and not the evaluation of a number of site-specific considerations.

3. On page 53, (third paragraph, first sentence) the authors claim that neural networks are used to approximate processes in the same manner as regression analysis. This is true of some neural networks and although many ANNs are evaluated against classical regression techniques, this does not apply to *all* networks.

4. (top of page 54) The authors make reference to "ten to twelve" (depending on the WMU of interest) parameters that were ranked as the most sensitive parameters for the majority of modeling scenarios for the two-tiered approach" and then state that "10 EPACMTP parameters were selected to develop neural networks". The box on the same page claims, "the Agency identified the top 12 most sensitive parameters for Industrial solid waste modeling scenarios" and then states, "of the top 12 parameters, 7 were identified that represent the most sensitive". This should be re-written (see comments on page 54).

5. (page 55, section 5.2) The authors finally reveal that the ANN selected for this investigation is a "feedforward, backpropagation neural network with one hidden layer". This should be revealed much earlier in the document, as references to the back-propagation of errors during training would make more sense.

6. (p.56) A figure similar to this would be helpful for each of the four neural networks developed in this work, since each network contains a slightly different set of inputs and outputs. If the reader thoroughly reads Appendix A, they would realize that (three?) of the ANNs posses two output values (log10 ave. conc., and log10 peak conc.), however, at this point in the document, the reader has been told that the output for each network contains a single groundwater well concentration converted to a DAF value.

7. (pages 60-61) Use different symbols/notation to distinguish between log peak concentration output generated by the ANN and that predicted by the EPACMTP model.

8. Note that – "the maximum 30-yr average well concentration (log ave. conc.)" (last bullet, middle of page A-7) is not the same as the "average peak 30-year concentration" mentioned in the middle of the same page.

9. (page A-15) The number of eons doesn't really "optimize" training time. It simply cuts down on the amount of data that is saved, presented, and/or printed.

10. (page A-27) The two graphs of Figure A.2.8. should be plotted on the same axes (in the same format that was used throughout the remainder of the document); and more than three data points should be used for illustrating the predictive capability of the EPACMTP. How was the neural network (used to produce the curve on the right hand side of Figure A.2.8.) trained? (on what data? how many data points? for what MWU? number of hidden nodes? convergence criteria?)

11. (page A-30)

> *"Preliminary analyses indicated that when values outside the training range (0th to 10th and 90th to 100th percentile OSW) are input to the trained neural networks, the neural networks recognized the value was out of the range of the input values."*

The backpropagation algorithm does not have a feature that enables it to recognize outliers or out-of-range input parameters. This is a very nice pre-processing feature of the IWEM graphical interface and should not be attributed to the ANN. In fact many references to the neural network method could be changed to the more general "Tier 2 model" as is done in the IWEM Users' Guide.

12. Table A.2.7 on page A-31 is more confusing than helpful. What needs to be said is described in the last paragraph on page A-30.

13. (page B-3) The equation that computes leachate flux through a hole in the geomembrane for which there is poor contact between the geomembrane material and the low-permeability soil, should be and not .

14. (p. B-17) The authors refer to "Data from the Florida study indicate….."
What Florida study?

15. (page B-9 through B-13) Figures B-1, B-2 , B-3, B-4 and B-5 are a bit confusing. Since the tests conducted consisted of "no holes" or "1000 holes" and did not consider intermediate ranges, a table might provide a better format for presentation of the results.

Contact	No holes	1000	Clay liner
	Leachate rates		
Poor			
Good			
Perfect			

16. (Appendix C) Axes on all the Figures should be labeled. Figure C-2 is identical to C-11. Should Figure C-2 contain histogram information for the infiltration rates with a single clay liner for landfills instead of waste piles?

APPENDIX C

ORIGINAL COMMENTS FROM LEAH ROGERS

Review of EPA Industrial Waste Management Evaluation Model (IWEM)

Contents:

A. Overview

Overall I believe this is a well-planned and executed project which should be of considerable use to those designing, approving, and evaluating facilities for handling industrial solid waste. The text has a good flow to it with concise description. The IWEM software is straightforward to

use, fast calculating and well documented. The underpinnings of the ANN formulation are carefully described and appropriate to this application.
In the following sections I make suggestions that may help users to more easily grasp what has been done on this project as well as document areas where I would have appreciated some clarification. In particular, there is a good level of ANN training complexity and thoroughness. Congratulations to those who have had the fortitude and discipline to carry out such an ambitious vision. This is a well-formulated, proactive outreach by EPA, which employs the sophistication and expertise of the combined fields of subsurface transport modeling, uncertainty analysis, and ANN technology. This outreach effort is packaged in a way that can be useful to those who do not have such a range of expertise but are in need of such insights.

B. Users' Guide to IWEM EPA 530-R-99-003

Introduction
One aspect that may be helpful to include is a definition paragraph on what a waste management unit is and specifically what the four types considered by the Tier 1 and Tier 2 analyses are. The four types are listed on page 2 but clarification of what distinguishes these units from each other and references to where they are defined in more detail would be useful.

The third paragraph is a good explanation of who will be likely users of the IWEM computer program. Another interesting aspect of motivation that could be included here is a brief discussion of economic issues. For example, why don't we use the most conservative liner for a WMU because prevention of contamination is often less expensive than remediation? What is the relative cost of these liners or how much difference in cost is there between say between a single liner and a more conservative composite liner. What have been some of the environmental and economic consequences of liners that have failed or overdesign of liners?

Table 1.1 page 4
What are the assumptions about the range of permeabilities of the single clay liner and composite liner? Perhaps there could be a pointer here to references about this issue.

Pg. 5: Note not all systems use report generation interchangeable with printing of results. See discussion below pg. 38 & 60.

1.3 2nd paragraph: "EPA used ranges of parameter values that result in a high estimate of risk"è how high?

Pg. 6: Good clarification of assumptions.

Pg. 13: Just curious: What motivated the cap on leachate concentrations less than or equal to 1,000 mg/L?

Pg. 19: Good outline of action to encourage user's variation of depth to water and aquifer thickness. Last Paragraph: What is a general range of radial distances to down-gradient monitoring well used by different state regulatory agencies? How does this range compare to ranges and defaults in table 4.2-4.5?

Pg. 20: Excellent to label a warning of uncertainty regions for parameter settings. Very good safety feature.

Pg. 38 & pg. 60: Report and Print Issue.
In the National Evaluation Summary and the Location-Adj Evaluation Summary the online text could add after the phrase "You may choose to print the results and exit this program" something like " To print results click on the report button at the bottom of the screen. Many systems do not automatically connect report with printing of results. I myself as a MAC user kept looking around for print or report icons, of course it is mentioned in the manual, but this would make the software more manual independent.

Pg. 53: It could be useful to have some justification examples here.

IWEM Interactive Model

Overall I found the software straightforward to step through the processes. Installation: Nice welcome, helpful defaults, installation and uninstallation methods consistent with industry standards.

Definition boxes:
Again WMU could use more definition here

Location Adjusted Evaluation:
Location parameters: defaults

As mentioned in the above section it might be useful to have some example justifications for parameters to indicate for archival purposes what degree of information is helpful. Also more completeness of steps in some of the windows would be helpful, for example description of hitting the report button below in order to get the print and report icons.

I experienced some freezing up of the system, perhaps due to my unfamiliarity with Windows (I am a Macintosh user primarily)

C. Technical Background Document EPA530-R-99-002 (ANN Background)

Overall: I like the impact of using a conservatively chosen DAR (90th percentile). Looks pretty clean, I notice several inconsistencies in the Dec 16 version have been corrected on the April 16 version.

Introduction:
Good concise overview of the two-tiered approach, discussion of uncertainty, and pointers to main Guidance. A particularly important point is the existence of Tier 3 possibilities.

Overall Modeling Strategy:

2.1. pg. 4. It might be helpful to list the three liner designs in the last sentence here with a pointer to their being discussed in more detail in section 2.1.2.

2.1.2. pg. 7
It would be interesting to have some brief summary, perhaps quoted from the main EPA Guide, about what types of clays are recommended to reach the 1 x 10 -7 cm/sec hydraulic conductivity levels, how difficult it is to insure an even 3 ft layer, or other interesting issues about quality and consequences of liner construction.

2.2.2   Basis for Use of the 90th Percentile
I read this paragraph as the EPA selected the 90th percentile output of the ground-water fate and transport modeling for this guidance but not that the 90th percentile is a standard with EPA for any Monte Carlo or other stochastic approach. You might wish to comment on whether using the 90th percentile is a standard recommended by the EPA and Science Advisory Board

or whether there is often a range over which the EPA recommends analysis. This would be a good place to discuss any studies where you may have examined variations between 85-95 percentile or observed how rapidly the percentiles change.

2.3.1 Overview of Neural Networks
Pg. 10: 1st paragraph, Correct spelling of reference (Rizzo and Dougherty, 1994).

3rd paragraph, One difference between neural networks and regression analysis which could be discussed here it that anns do not require an a priori model or prespecified curve type which the data will be fit to. Instead the ann empirically develops its own representation of the data expressed by the weights.

Pg. 11: This is a very concise and eloquent backprop description. You may wish to note that you are describing backpropagation neural networks that form the majority of applications; however, this does not pertain to other types of neural networks. This could be tied into the description of backprop and conjugate gradient training in the appendix, note the comments below for the appendix pg. A-15.

Pg. 12: 4th paragraph. In the discussion of over-fitting it may be helpful to discuss how the training set is usually such a small sampling of the overall range of possibilities or search space and over-fitting is where network weights get too specialized on idiosyncratic features of the training set and thus has a lower generalization performance (i.e. performance on the larger search space beyond the training set).

Pg. 12: last paragraph: It would be good here to have a bit more description of sensitivity analysis of output to input value changes. I believe you are referring to input value changes not changes in which type of input you are using.

3.2.3
pg.27 Good to see you have included the complexity of a non-linear concentration dependant isotherm.

3.3 EPACMTP
pg. 28: Which parts of the contaminant transport component use analytical techniques and which use numerical?

3.3.3
pg. 33: It would be interesting to have a list of the 52 EPACMTP input parameters here next to the list of 28 parameters just for comparison.

pg. 34: 1st paragraph: How about a list of the 10th to 90th percentile values for the 28 parameters or a pointer to where it is discussed in more detail? For instance, the median aquifer thickness seems quite thin and it would be interesting to see the range used in the deterministic sensitivity analysis.

pg. 36: 2nd paragraph, last sentence: Again how about identifying where the number of parameters in the subset are discussed in more detail.

pg. 39: Table 3-5 and 3-6 Check for consistency about whether second and third words of parameter descriptions are capitalized: example Depth of Unsaturated Zone is also spelled Depth of unsaturated zone. Also variation in Angle of Well off of Plume Centerline.

Table 3-7 pg. 43: Consider adding the word "only" into the phrase "ponding depth for surface impoundments [only]".

Pg. 45: first full sentence: while is misspelled in "wile maintaining the desired accuracy".

pg. 50: Figure 4-1 Note spelling of radius.

5.2
Pg. 55: The discussion of Figure 5-1 states "The output layer consisted of the ground-water well concentration which are then converted to a DAF." The concentration in the singular does not match the noun "are" in the plural, and Figure 5-1 describes two concentrations, an average concentration and a peak concentration.

Pg. 59: It seems the table called out as Table 5-7 is labeled as Table 5-1 on page 62.

Pg. 62: Table 5-1 Why are there so few landfill training data sets?

Pg. 63: Could you clarify how the testing and validation data sets relate to each other and if there is any overlap between them. Also consider adding a pointer to the appropriate appendix. Will you consider adding more landfill and land application training data sets and doing more training to further gain "incremental gains in predictive ability that may be realized through additional neural network training"?

Pg. A-2: A.2.1. Again clarification about whether there is any overlap between test and validation data sets would be helpful. Also on the last line there is a space gap between additional secondary in the last line on the page A-2 and test data on pg. A-4. Figure A.2.1. seems to suggest that the training data matrix is a subset of 30% of the validation data matrix and that doesn't seem likely as the training set is so much larger than the validation set.

Tables A.2.1-5 The input parameter term RADIS does not match the term listed on pg. A-7 RADIUS.

Pg. A-7 A.2.1.1. The two EPACMTP output parameters used to train the anns are listed in the first sentence of the middle paragraph as the peak well concentration and the maximum 30-yr average well concentration. The last sentence in the middle paragraph states "Therefore, the landfill neural network did not consider DOC as an input parameter and did not use the average peak 30-year concentration as an output parameter." Is the maximum 30-yr average well concentration then the average peak 30-year concentration?

Pg. A-7: The last paragraph has the phrase "representing the of seven input parameters." Missing word?

Pg. A-9 Good discussion of using histograms to make sure input values in the training were represented a balanced distribution. Also you have used a nice range of methods to develop additional data sets.

Pg. A-10 It would be helpful to include more discussion of logic behind the creation of additional data samples. For example the group 1 data samples appear to be created to add in test data which had not been well predicted by the networks (i.e. higher residuals) to the training data.
The discussion of the Group 4 data samples is good. Overall one has the sense from the conclusions herethat the waste pile and land application unit networks benefited from what you learned during training the landfill and surface impoundment nets and the former two nets have better summary statistics (pg. 62). It's not clear that you took all that you learned back into the training of the landfill and surface impoundment nets to get

the best performance you could from them.

Another point, for the nets with two outputs, did you consider dividing a network into two networks one trained for each of the outputs; this increases the ratio of training examples to network weights and can help performance.

Pg. A-14 Initialization: Good point raised about the initial settings having a "significant affect on overall performance". You state you did not perform an analysis to determine the "optional" initial settings. Did you mean optimal instead of optional? Did you vary the initialization weights over some range in different training?

Pg. A-16 Terminology Question: I would refer to these two types of training methods as variations of learning and that the conjugate gradient training is still used in a backpropagation network. Is that your use of the terminology? If so it might be good to clarify that here. One might just call the first training backpropagation with steepest descent learning and the second backpropagation with conjugate gradient learning.

Also my understanding of the conjugate gradient method is that the second derivative of the error surface is used to signal a point of decreasing returns on the training and at this point a step in a direction perpendicular to the error gradient is taken, thus the name conjugate gradient. If this is what your algorithm is doing, I think this is an interesting point to give readers a physical sense of how the search proceeds and contrast this to the steepest descent gradient approach as the conjugate gradient goes downgradient until there is a flat spot and then jumps perpendicular if it looks like there is stagnation. Note this is a powerful approach to avoid local minimums in the search space. These points would help explain the why behind your statement that the conjugate gradient training is "generally more accurate for optimizing weights". Note in the text this statement has an extra "a" before the more accurate, need remove it or add "method" after accurate.

Pg. A-14 Did you ever use less than 10 hidden nodes, if so how was the performance? Usually a simpler net is preferred so there are less network weights and the number of examples goes further.

Pg. A-23 Figure A.2.3 What physically do the oscillations mean in Log of peak concentration at the higher observation numbers?

Pg. A-23 First paragraph. The phrase is used " a trained neural network that used many additions of training data sets". How many additional examples were used?

Pg. A-27: Figure A-2-8 Why are there only three data points from EPACMTP data plotted here?

Pg. A-29: Is evaluation of the ann's performance outside the 10th to 90th percentiles planned to be accomplished before this model is released to a wider audience?

Pg. A-34 LFNN training appears to have good generalization despite the relatively few training examples. It is possible this is because the ann was being asked to predict one output.

Pg. A-44: Perhaps there is less anxiety producing or confidence lessening terminology to use than good and bad here. Consider concepts such as dense or sparse coverage or well/poorly sampled.

Pg. A-48: I'm still just missing something here, it's not clear to me why the surface impoundment curves have such strong oscillations.

Pg. A-53: This seems to be the ann's poorest validation performance of the four types of waste units. Again I would be curious if training to one output at a time would be a quick way to see if some improvement could be made. For example use 2747 training examples to train for log of peak conc and then use them to train for log of average conc.

**It would be nice to have the number of inputs and number of output reviewed inthe summary tables of final ann features for each of the four types.

Pg. A-59: With all this appending three times it would be good to have footnotes in the summaries of number of training runs about how many were unique runs. If they are lumped into the training runs too many times the summary statistics may be misleading. It's one thing to append them to the training set to help "balance data combinations" as you say, but it would be good to clarify if this is not inflating the actual number of unique training runs.

Pg. A-60: Interesting concept of a chemical validation set. Even though

WPNN-A did not win out this may be a type of metric you wish to keep in mind for next generations of this tool.

Overall on the anns: As you have stated the performance is better on the last two nets and poorest on the surface impoundment's nets. Again, perhaps you have plans to go back into the first two with the deeper experience with adding additional training data sets.

Pg. A-83: This is a significant effort and reflects much progress. Continuing to refine the methodology is an important investment in increasing the dependability and acceptance of such visionary tools.

Pg. D-1: Again it may be appropriate here to differentiate between the type of neural network referred to as backpropagation network and the variations in learning.

Pg. D-2: Under Feed Forward Propagation it might be more accurate to call this a neural network process rather than method because it is something done with an entity rather than an entity itself.

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EDUCATION

Ph.D., Applied Mathematics, University of California, Davis, 1971.

M.S., Biomathematics, California State University, Fresno, 1967.

B.S., Mathematics and Physics, California State University, Fresno, 1966.

EXPERIENCE

1998 to Present	Project Performance Corporation Vice President Environmental Risk and Security Responsible for coordination of risk-related activities of the corporation.
1996 - 1998	Informatica International, Inc. Chief Operating Officer Responsible for operation of a professional services organization providing information, engineering and environmental support to government and private sector clients.

1976 - 1996	Oak Ridge National Laboratory Director, Center for Risk Management and Head, Risk Analysis Section Responsible for coordination of health and environmental risk analysis activities at Oak Ridge National Laboratory
1996	Corporate Fellow at Oak Ridge National Laboratory. This designation is made on a limited basis to recognize exceptional technical achievements in science and engineering.
1991 - 1996	Director, Center for Risk Management. Responsible for coordination of health and environmental risk analysis activities at Oak Ridge National Laboratory.
1991 - 1996	Head, Risk Analysis Section, Health Sciences Research Division, Oak Ridge National Laboratory. Responsible for health risk assessment activities within the Health Sciences Research Division.
1984 - 1991	Coordinator, Office of Risk Analysis, Health and Safety Research Division, Oak Ridge National Laboratory. Responsible for coordination of health risk assessments and related research and development.
1977 - 1984	Leader, Exposure Analysis Group, Health and Safety Research Division, Oak Ridge National Laboratory. Responsible for development of environmental transport methodologies for toxic chemicals.
1976 - 1977	Research Staff, Environmental Sciences Divisions, Oak Ridge National Laboratory. Performed radiological assessments and worked in theoretical population ecology.
1974 - 1976	Assistant Professor, Department of Mathematics, University of Tennessee. Taught courses in applied mathematics and computer sciences.
1971 - 1974	Assistant Professor, Department of Mathematics, Vanderbilt University. Taught courses in applied and engineering mathematics.
1966 - 1968	Research Engineer, Jet Propulsion Laboratory, California Institute of Technology. Computer analysis of space craft flight simulation.

PROFESSIONAL ACTIVITIES

Editorial Boards

Editor-in-Chief, *Risk Analysis: An International Journal*, 1983 - Present.

Editorial Board, *Health and Environmental Toxicology*, 1989 - Present.

Editorial Board, *Toxicological and Environmental Chemistry*, 1989 - Present.

Editorial Board, *Toxicology and Industrial Health*, 1990 - Present.

Editorial Board, *Journal of Hazardous Materials*, 1990 - Present.

Editorial Board, *Critical Reviews in Environmental Science and Technology*, 1991 - Present.

Editorial Board, *DOE Risk Management Quarterly*, 1994 - Present.

Society Memberships

President, International Society of Risk Analysis, 1991.

Fellow, International Society for Risk Analysis, 1992 - Present.

Member, International Society of Exposure Analysis, 1991- Present.

Member, American College of Toxicology, 1990 - Present.

Member, Society of Toxicology, 1990 - Present.

Distinguished Service Award, Society for Risk Analysis, 1984.

Senior Research Fellow with Energy, Environment, and Resources Center at the University of Tennessee, 1990 - Present.

President, East Tennessee Chapter of the Society for Risk Analysis, 1988.

National Academy of Sciences Panels

National Academy of Sciences Committee on Environmental Management Technologies, 1995

National Academy of Sciences Workshop to Review Risk Management in the Department of Energy's Environmental Restoration Program, 1993 - 1994.

National Academy of Sciences Committee on Remedial Action Priorities for Hazardous Waste Sites, 1991 - 1993.

National Academy of Sciences Board on Radioactive Waste Management Committee to Review Hanford Single Shell Tanks, 1989 - 1993.

National Academy of Sciences Board on Radioactive Waste Management Committee to Review TRU Waste at Idaho National Laboratory, 1989 - 1993.

National Academy of Sciences Committee on Biomarkers for Immunotoxicology, 1989 - 1992

National Academy of Sciences Consultant to Committee on Animals As Monitors of Environmental

Hazards, 1989.

National Academy of Sciences Subcommittee on the Use of Pharmacokinetics in Risk Analysis, 1986 - 1987.

National Academy of Sciences Symposium on Managing the Problem of Industrial Hazards: The International Policy Issues, 1989.

National Academy of Sciences Advisory Panel on Markers of Exposure to Toxic Substances: National Monitoring of Human Tissues, 1988 - 1989.

National Advisory Boards

Advisory Board of the Earth 2020--Center for Environmental Policy at the University of Virginia.

Science Advisory Board, National Center for Toxicological Research, Food and Drug Administration, 1986 - 1991

Scientific Advisory Panel on The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) for the US Environmental Protection Agency, 1990 - 1994.

Advisory Panel, Department of Energy, National Environmental Restoration Prioritization Program, 1989 - Present.

New York City Department of Environmental Protection, Technical Advisory Committee on the Land Base and Sewage Sludge Disposal Program, 1989 - 1992.

Environmental Protection Agency Review Panel for Land Application of Pulp and Paper Mill Sludge, 1991.

National Academy of Sciences Workshop on Single Scenario and Population Distribution Estimates of Exposure: Applications and Implications in Risk Assessments, 1992.

Scientific Advisory Board, Chemical Industry Institute of Toxicology, 1991 - 1992.

Environmental Protection Agency Review Panel for Dermal Exposure Assessment, 1991.

World Health Organization Consultation on Tolerable Daily Intake from Food of PCDDs and PCDFs, 1990.

Chairman, Office of Science and Technology Policy Task Force on Risk Analysis, 1985 - 1990.

Advisory Panel, Clean Sites Remedy Selection Project, 1989 - 1990.

New Jersey State Department of Health Advisory Panel on Superfund Sites, 1988 - 1990.

Environmental Protection Agency Review Panel for Cancer Risk Assessment Guideline Revision, 1989.

W-170 Peer Review Committee for Proposed EPA Regulations Municipal Sewage Sludge, 1989.

Review Panel, Resources for the Future Study of Uncertainty in Risk Analysis, 1989.

American Industrial Health Council Study Group on Presentation of Risk Assessments, 1988-1989.

Planning Committee and Chairperson, Biological Data for Pharmacokinetic Modeling and Risk Assessment, 1988.

National Science Foundation Advisory Panel for Selection of National Science and Technology Centers, 1988.

National Cancer Institute, US - Japan Cooperative Cancer Research Panel, 1987.

Environmental Protection Agency Peer Review Panel on Interim Methods for Development of Inhalation Reference Doses for Systemic Toxicants, 1987.

American Industrial Health Council, Delivered Dose Work Group, 1987 - Present.

Risk Science Institute Panel on Risk Communication and the Public's Right to Know, 1986.

Environmental Protection Agency Review Panel on Biologically Motivated Mathematical Models in Cancer Risk Assessment, 1986.

Conservation Foundation Panel on Environmental Health: Cross Media Perspectives, 1985-1986.

National Science Foundation Task Force on Risk Analysis, 1985.

National Science Foundation Task Force on Risk Assessment Methods for Environmental Applications of Biotechnology, 1985.

American Industrial Health Council Committee on Risk Analysis, 1985.

US - Japan Task Force on Risk Management, 1984.

US - Japan Fusion Cooperation Program on Tritium Radiobiology, 1984.

US Army Review Board on Hexachlorethane Smoke, 1984.

DOE/EPA Risk Assessment Focus Group, 1993.

Advisory Panels

Duke University Medical Center Waste Disposal Advisory Group, 1993-1994.

Advisory Panel for the Office of Technology Assessment on Research on Risk Assessment Methodology for Chemical Carcinogens, 1992 -1993.

Gas Research Institute Project Advisory Group, 1992 - 1994.

Science Advisory Panel, Chemical Industry Institute of Toxicology, 1991.

State of Maryland Advisory Panel on the Maryland Power Plant Research Program, 1988 - 1990.

Science Advisory Board, New Jersey Governor's Panel on Health and Environmental Issues, 1988 - Present.

Medical Research Council of Canada Peer Review of Canadian Environmental Health Directorate, 1989.

New Jersey Clean Air Council, 1989.

Advisory Panel on Municipal Waste Incineration, Nashville Metropolitan Health Department, 1989.

Federal Task Force to Investigate Offsite Contamination at Oak Ridge Reservation, 1985 - 1989.

State of Connecticut Advisory Panel on Hazardous Air Pollutant Control Program, 1988.

Risk Management Advisory Panel, State of California South Coast Air Quality Management District, 1987.

Review Panel for the Risk Assessment of the Ontario Waste Management Hazardous Waste Incinerator, 1985 - 1987.

City of Los Angeles Advisory Committee for the Risk Assessment of the LANCER Incineration Project, 1986 - 1987.

Planning Committee - Carcinogenic Risk Assessment: The Chlorinated Solvents, 1986 - 1987.

Review Panel for Pharmacology Program at Pennsylvania State University Medical School, 1986.

Expert Panel on PCB Contamination in Bloomington, Indiana - Incineration Subcommittee, 1993.

Adjunct Faculty Member, Environmental Systems Engineering Department, Clemson University.

Adjunct Faculty Member, Life Sciences Department, University of Tennessee, 1994.

<u>Congressional Testimony</u>

House Committee on Science, Space and Technology, Subcommittee on Environment, "Use of Risk Analysis for Prioritization of Environmental Spending" 1991.

U. S. Senate Committee on Environment and Public Works, Subcommittee on Superfund, Waste Control and Risk Assessment, “The Role of Risk Assessment in Superfund,” April 5, 1995.

CONFERENCES ORGANIZED SINCE 1985

Course Director, Society for Risk Analysis Course on Carcinogenic Risk Analysis, 1985 - Present.

Co-Director, NATO Advanced Study Institute on Risk Assessment for Environmental Applications of Biotechnology, 1987.

Director, NATO Advanced Study Institute on Biologically Based Methods in Cancer Risk Assessment, Corfu, Greece, 1988.

Co-Director, Pan American Health Organization Workshop on Environmental Risk Analysis, Havana, Cuba, 1988.

Co-Director, Pan American Health Organization Workshop on Risk in Developing Countries, Mexico City, Mexico, 1988.

Co-Director, Workshop on Risks of Toxic Substances in Developing Countries: Implications for Women and Children, Bangkok, Thailand, 1988.

Director, Society for Risk Analysis Course on Carcinogenic Risk Assessment, Washington, DC, 1988.

Co-Director, US-India Workshop on Environmental Risk Analysis, New Delhi, India, 1989.

Co-Director, Workshop on Risk Assessment for Municipal Waste Combustion: Deposition, Food Chain Impacts, Uncertainty, and Research Needs, Cincinnati, Ohio, 1989.

Co-Director, Workshop on Reauthorization of Superfund, Gatlinburg, Tennessee, 1989.

Director, Society for Risk Analysis Course on Carcinogenic Risk Assessment, Washington, DC, 1989.

Chairman, Air Quality and Environmental Risk, Pittsburgh, Pennsylvania, 1990.

Director, Society for Risk Analysis Course on New Directions in Risk Assessment, Washington DC, 1990.

Chairman, Society for Risk Analysis Annual Meeting, New Orleans, 1990.

Co-Director, NATO Advanced Research Workshop on the Use of Biomarkers in Assessing Health and Environmental Impacts of Chemical Pollutants, Luso, Portugal, 1992.

Course Director, Risk Assessment Seminar, Department of Energy, 1992.

Director, National Workshop on Critical Issues in the Cleanup of Federal Facilities, Knoxville, Tennessee, 1993.

Co-Director, Public Health Assessment Training Workshop, Porto, Portugal, 1993.

Course Director, Society for Risk Analysis, "New Horizons in Risk Assessment," August 1994.

PLENARY ADDRESSES

U.S. - Japan Conference on Risk Assessment and Risk Management, 1987.

13th Symposium on Aquatic Toxicology, "Aquatic Toxicology and Risk Assessment," 1989.

Dioxin 89, "Dioxin" Research Needs for Risk Assessment," 1989.

Health Physics Society, "A Scientific View of Risk Assessment," 1990.

Dioxins and Dibenzofurans Symposium, "Human Exposure to Dioxin," 1990.

National Groundwater Association, "Effectiveness of Groundwater Remediation," 1992.

National Council on Radiation and Protection, "Below Regulatory Concern," 1993.

International Congress on the Health Effects of Hazardous Waste, "Hazardous Waste Cleanup at Federal Facilities: The Need for an Integrated Policy," 1993.

MAJOR INVITED PRESENTATIONS SINCE 1986

National Institute for Environmental Science, Hyderbad, India, "Use of Wood in Developing Countries," 1986.

Conservation Foundation, "The Nature and Extent of Cross-Media Pollution," 1986.

Harvard University, "Environmental Transport of Radionuclides in Water and Food," 1986.

Risk Science Institute, "Federal Initiative in Risk Analysis," 1986.

Brookings Institute, "Risk Analysis in Regulatory Decisions," 1986.

State of Maine, Board of Environmental Protection, "Risk Analysis/Risk Management," 1986.

Centennial Celebration Sigma XI, Washington, DC, "Risk Communication," 1986.

National Academy of Sciences, "Interspecies and Dose-Route Extrapolations" 1986.

U.S. Environmental Protection Agency, "Use of Pharmacokinetics in Risk Assessment," 1986.

Agency for Toxic Substances and Disease Registry, "Risk Communication: A Problem in Process, Not Information Transfer," 1986.

American Industrial Health Council, "Interspecies Scaling," 1987.

Environmental Protection Agency, "Initiation and Promotion in Pharmacodynamics," 1987.

U.S. - Japan Cooperative Cancer Research Program, "Mathematical Modeling in Risk Assessment," 1987.

Banbury Conference on New Directions in the Qualitative and Quantitative Aspects of Carcinogen Risk Assessment, 1987.
Only One Earth Forum, Rene Dubos Center for Human Environments, 1987.

Environmental Protection Agency, "Cancer Risk Management by Federal Agencies," 1987.

Rene Dubos Center for Human Environments, "The Food Chain as a Source of Toxics Exposure," 1987.

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Connecticut Department of Health and Environment, "Pharmacokinetics of Perchloroethylene," 1988.

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"Prediction of Carcinogenic Potency from Toxicological Data," Guadalajara, Mexico, 1989.

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National Institute for Standards and Technology, "Comparative Potency Approach to Risk Assessment of PAHs," 1989.

US Geological Survey, "Decision Process at Superfund Sites," 1990.

Institute Superior of Health, "Pharmacokinetics in Risk Assessment," Rome, Italy, 1990.

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Oak Ridge National Laboratory Senior Planning Group, "Center for Risk Management," Oak Ridge, Tennessee, 1991.

Chemical Hazards Training Seminar, Health and Welfare Canada, "Multimedia Exposure Assessment," 1991.

Department of Mathematical Sciences Meeting, Johns Hopkins University, "Dimethylnitrosamine - Induced Hepatocarcinogenesis in Rats: A Theoretical Study," 1991.

Environmental Remediation, "Health-Based Cleanup Goals at Hazardous Waste Sites: Implications for Risk Management," 1991.

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Robert Wood Johnson Medical School, "Risk Analysis and Priority Setting for Environmental Policy," 1991.

American College of Toxicology, "Cell Proliferation: Application to Carcinogen Risk Assessment," 1991.

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Lake Charles Louisiana Committee for Environmental Action, "Global Chemical Pollution," 1991.

Rutgers University, "Risk Assessment and Prioritization of National Environmental Policy," 1991.

International Society of Exposure Analysis Annual Meeting, "Dosimetrics for Use in Risk Analysis," 1991.

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Vanderbilt University's Eckenfelder Seminar, "Use of Risk Assessment in Setting Priorities for Superfund Sites," 1992.

National Academy of Sciences, "Priority Systems Application," 1993.

International Congress on the Health Effects of Hazardous Waste, " Hazardous Waste Cleanup at Federal Facilities: The Need for an Integrated Policy", Atlanta, Georgia, 1993

Industry Forum, "Hazardous Waste Cleanup at Federal Facilities: The Need for an Integrated Policy," Oak Ridge, Tennessee, 1993.

Oak Ridge Chamber of Commerce, "Center for Risk Management", Oak Ridge, Tennessee, 1993.

National Conference on the Federal Cleanup, "The Need for a National Hazardous Waste Policy for Federal Facilities," 1993.

U.S. Department of Energy, 29th Annual Meeting of the National Council on Radiation Protection and Measurements, "BRC Levels for Chemical Exposures: Radiation Science and Societal Decision Making Case Study Session: Below Regulatory Concern," 1993.

EMAC Subcommittee Meeting, "PEIS-ER Human Health Risk Installation-level Approach," Hyatt Regency Hotel, Chicago, Illinois, 1993.

EMAC Subcommittee Meeting, "PEIS (Programmatic Environmental Impact Statement) Waste Management Risk Assessment, Hyatt Regency Hotel, Chicago, Illinois, 1993.

Waste Management Symposia, Inc., Tucson Convention Center, "Risk Assessment for the Delayed Retrieval of Transuranic Waste", Tucson, Arizona, 1993.

American Society for Mechanical Engineers, Solid Waste Processing Division, Eastern Chapter Meeting, Tampa Florida, "Mercury: Environmental Partitioning and Human Exposure" 1993.

Fifth Meeting of the Risk-Based Standards Working Group, "Use of Oncogenic Models to Study the Cancer Process", Washington, DC, 1993.

Future Land Use Working Group Meeting, "Land Use and Integrated Risk Management", Rockville, Maryland, 1993.

U.S.-Department Of Energy Environmental Restoration Programmatic Environmental Impact Statement Risk Assessment Model Review Tutorial Meeting, "PEIS - Environmental Restoration and Waste Management", Oak Ridge, Tennessee, 1993.

Health Effects Research Laboratory (HERL) Symposium on Biological Mechanisms in Quantitative Risk Assessments - Cancer Risk Assessment Session, "Cancer Risk Assessment: What Have We Learned from Biologically-Based Models", 1993

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Vanderbilt University, "Hazardous Waste Cleanup at Federal Facilities: The Need for an Integrated Policy", Nashville, Tennessee, 1993.

U.S. Department Of Energy's EM-PEIS Risk Assessment Model Review Workshop, "PEIS Risk Assessment Modeling", Rockville, Maryland, 1993.

Waste Management 1994, "Human Health & Ecological Risks from Environmental Restoration and Waste Management Activities", Tucson, Arizona, February, 1994.

Ohio State University, College of Nuclear Engineering, Interdisciplinary Lecture Series, "Applications of Risk Assessment to Cleanup of Contaminated Department of Energy Sites", Columbus, Ohio, February 17, 1994.

Waste Management Symposium, "Risk Assessment for the Retrieval of Transuranic Waste", Tucson, Arizona, February 1994.

The 208th American Chemical Society National Meeting, "Health Risks Associated with Air Emissions from MSW Combustion", Washington, DC, 1994.

DOE-EM-6 Tulane/Xavier Consortium for Environmental Risk Evaluation Team Meeting, “Public Unit Risk Approach for Cumulative Impacts Analysis”, Oak Ridge, TN, June 13, 1994.

National Research Council Meeting, “PEIS: Decontamination and Decommissioning of Facilities”, Washington, DC, June 16, 1994.

Presentation to the Russian Delegation, "Center for Risk Management," Oak Ridge National Laboratory, Oak Ridge, Tennessee, August 9, 1994.

Waste Management 1994, "Human Health and Ecological Risks from Environmental Restoration and Waste Management Activities", Tucson, Arizona, August 21-26, 1994.

Oak Ridge Model Conference (Waste Management and Environmental Restoration), "Risk Analysis and Environmental Restoration," Pollard Auditorium, Oak Ridge, Tennessee, August 23, 1994.

Eighth Annual Risk Assessment Court, Society of Risk Analysis, “New Horizons in Risk Assessment”, Arlington, VA, August 29-30, 1994.

1994 International Decontamination and Decommissioning Symposium, "Evaluation of Remediation Worker Risk at Radioactively Contaminated Waste Sites", Knoxville, Tennessee, 1994.

ORNL Risk Assessment Seminar, "Risk Assessment Issues Part I and II, Germantown, Maryland, 1994.

Clemson University, Environmental Engineering Graduate School Seminar, "Risk Communication and Stakeholder Involvement", Clemson, South Carolina, 1994.

EM-30 Meeting, "Waste Management Risk Assessment System", Washington, DC, 1994.

International Symposium on Assessing and Managing Health Risk from Drinking Water Contamination: Approach and Application, Rome, Italy, September 13-17, 1994.

Puerto Rican Initiative Meeting, “Energy Action Plan for Puerto Rico”, Oak Ridge National Laboratory, Building 3047, Oak Ridge, Tennessee, November 3, 1994.

Hamilton Laboratory Meeting, “Worker Health Risk Evaluation Methodology”, Cincinnati, Ohio, November 8,1994.

Department of Energy, “Worker Health Risk Evaluation Methodology”, DOE Trevion Building, Washington, D. C., November 9, 1994.

Annual Meeting, Society Risk Analysis, “Technologies and Contaminants Posing the Greatest Risk to Workers During Remediation of U. S. DOE Waste Sites”, Baltimore, MD, December 4-7, 1994.

Sustainable Energy Meeting, “Sustainable Energy Technology Opportunities for Puerto Rico”, The University of Puerto Rico, Mayaguez, Puerto Rico, December 16, 1994.

White House Council on Sustainable Development meeting, “A Framework for Sustainable Development in Puerto Rico, Washington, DC, December 21, 1994.

Association for the Advancement of Science, “Problems with Remediation of Contaminated Soils”, Atlanta Marriott Marquis, Atlanta, Georgia, February 18, 1995.

Chemical Risk Assessment Course, “Pathway Analysis for Chemicals Released to the Environment”, Kiawah Island Resort, Kiawah Island, South Carolina, February 28, 1995.

Environmental and Occupational Health Sciences Institute, “Human Exposure to Environmental Contaminants”, Rutgers University, Piscataway, New Jersey, March 9, 1995.

Harvard Center for Risk Analysis Symposium on Weighing the Risks, “Risk Tradeoffs in Superfund Policy”, Washington, DC , March 30, 1995.

Health Sciences Research Division Information Meeting, “Risk Analysis Section Overview’, Weinberg Auditorium, Oak Ridge National Laboratory, April 19, 1995.

ORNL Federal Facility Agreement (FFA) Technical Advisory Meeting, “Risk-Based Prioritization of Waste Management Activities”, May 19, 1995.

DOE meeting, “A Framework for Sustainable Development in Puerto Rico”, Washington, DC, May 29, 1995.

East Tennessee Chapter Meeting of the Society of Risk Analysis, “The Hazardous Waste Problem: What Should We Do?”, Science Applications International Corporation, Oak Ridge, Tennessee, June 22, 1995.

Russian 3rd Environmental Remediation Course, “Risk Assessment as a Tool for Environmental Restoration”, Pollard Auditorium, Oak Ridge, Tennessee, June 12, 1995.

Air Force Center for Environmental Excellence Meeting, “Capabilities Briefing to the Air Force Center for Environmental Excellence,” San Antonio, Texas, June 19, 1995.

National Research Council Panel on Priority Setting/Timing & Staging of Environmental Management Activities of the Committee to Evaluate the Science, Engineering, and Health Basis of the DOE’s Environmental Management Plan, “Priority Setting,” National Academy of Sciences Building, Washington, D. C., June 27, 1995.

Baseline Environmental Management Task Force, “Life-Cycle Risk Estimation”, Washington, DC, August 10, 1995.

DOE Environmetnal Restoration Headquarters, Center for Risk Management Program Review, Washington, DC, October 30, 1995.

Lockheed Martin Environmental Management Integration Team Meeting, “Common Approach to Risk Management,” Albuquerque, New Mexico, January 11, 1996.

Vanderbilt University, “Problems with Remediation of Contaminated Soils”, Vanderbilt University, Nashville, TN, February 26, 1996.

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BIOGRAPHICAL SKETCH AND BIBLIOGRAPHY

Donna M. Rizzo
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Education Institution and Location	Degree	Date Conferred	Field of Study
University of Connecticut, Storrs	B.S.	1984	**Civil Engineering**
University of Florence, Italy	N.A.	1985	Art and Archeology
University of California, Irvine	**M.S**.	1990	**Civil Engineering**
University of Vermont, Burlington	**Ph.D**.	1994	**Civil** & Environmental **Engineering**

Research and Professional Experience

1995-present	**Co-founder**, Subterranean Research, Inc., Burlington, VT.
1995-present	**Research Assistant Professor**, Department of Civil & Environmental Engineering, The University of Vermont, Burlington, VT. (currently on unpaid leave of absence)
1991-1994	**Research Assistant**, University of Vermont, Burlington, VT. *Research*: geohydrologic site characterization using artificial neural networks, optimal groundwater remediation design, highly-parallel implementation of numerical methods for geohydrological applications. Teaching assistant for ME 93 (Bioengineering) and ME 14 (Mechanics of Solids).
1992-1995	**Instructor**, Princeton Transport Code Short Course, with George F. Pinder, Stuart A. Stothoff, Joseph F. Guarnaccia, and George P. Karatzas.
1992-1994	**PC Laboratory Instructor**, IBM PC Applications in Ground Water Pollution and Hydrology Short Coarse, taught by Robert W. Cleary, Michael J. Ungs, and George F. Pinder.
1992-1994	**Participating Guest**, Lawrence Livermore National Laboratory, Livermore CA.
1987-1990	**Research Assistant and Graduate Teaching Assistant**, University of California, Irvine, CA. *Research*: mathematically modeling multi-phase flow and transport in the unsaturated zone with DBCP (a pesticide) present, development of knowledge based engineering systems for hazardous waste site evaluations. *Teaching assistant* for CE 172 (Hydraulics).

Awards

One of 15 people selected in a national competition to attend a 12-week workshop at the Advanced Computing Laboratory at Los Alamos National Laboratory, Spring, 1993; Graduate Teaching Fellow of the Year, University of Vermont, Department of Civil & Mechanical Engineering, 1990-1991; GPOP Fellowship, University of California, Irvine (Financed 100 % of M.S. Degree).

Recent Publications (Selected)

P.A. Sullivan, D.M. Rizzo and D.E. Dougherty, "Hierarchical artificial neural networks for regionalized cokriging", Proc. XII International Conference on Computational Methods in Water Resources, Vol. I, Crete, 1998.

D.M. Rizzo, and D.E. Dougherty, “Solving Groundwater Inverse Problems Using Artificial Neural Networks”, in (Aldama *et al.*, Eds.) XI Intl. Conference on Computational Methods in Water Resources XI, Vol.1, Computational Mechanics Publications, pp. 313-319 Cancun, Mexico, 1996.

D.M. Rizzo, and D.E. Dougherty, “Application of Artificial Neural Networks for Site Characterization Using ‘Hard’ and ‘Soft’ Information”, in (Peters *et al.*, Eds.) X International Computational Methods in Water Resources X, Vol. 1, Kluwer Academic Publishers, pp. 793-799, Heidelberg, Germany, 1994.

D.M. Rizzo, and D.E. Dougherty, “Characterization of aquifer properties using artificial neural networks: Neural Kriging”, *Water Resources Research*, 30 (2), pp. 483-497, 1994.

D.M. Rizzo, D.E. Dougherty and T.P. Lillys, “Site Characterization at LLNL Using Artificial Neural Networks”, Water Policy and Management: Solving the Problems, Proc. of the 21st Annual ASCE Conference of Water Resources Planning and Management Division, pp. 250-253, Denver, Colorado, May 23-26, 1994.

D.M. Rizzo, and D.E. Dougherty, “Design Optimization for Multiple Management Period Groundwater Remediation”, Water Resources Research, 32 (8), pp.2549-2561, 1996.

D.M. Rizzo, T.P. Lillys and D.E. Dougherty, “Comparisons of Site Characterization Methods Using Mixed Data”, in (Shackelford, et al., Eds.) Uncertainty in the Geologic Environment: From Theory to Practice, Vol. 1, ASCE Proc. for the 1996 GED Specialty Conference, pp. 167-179, Madison, Wisconsin, 1996.

D.M. Rizzo, and D.E. Dougherty, “Characterization of Porous Media using ‘Hard’ and ‘Soft’ Information”, in (Russell et al., Eds.) IX International Computational Methods in Water Resources IX, Vol. I: Numerical Methods in Water Resources, CMP/Elsevier, pp. 449-455, Denver, CO,1992.

D.M. Rizzo, “SCANN Site Characterization using Artificial Neural Networks.”, Version 1.0, Software based on this approach is being incorporated by the University of Vermont and Applied Research Associates Inc. into a real-time cone penetrometer system funded by Tyndall Air Force Base. Software, User’s Guide available through the University of Vermont, Burlington, VT, 1994.

J.L. Adler, D.M. Rizzo, and S.G. Ritchie, SITE Site Investigation and Training Expert Advisor. Version 2.0 User's Manual and Reference Guide available through the California Department of Transportation, Sacramento, CA, 1990.

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EDUCATION:

¥ Doctor of Philosophy Hydrogeology	Stanford University Stanford, California	August 1992
¥ Master of Science Hydrogeology	University of Illinois Urbana-Champaign	May 1979
¥ Bachelor of Science Geology/Urban Studies Magna cum Laude	Southern Methodist University Dallas, Texas	May 1977

PREVIOUS RESEARCH EXPERIENCE:

1979-Present **Hydrogeologist-** Geosciences and Environmental Technologies Division, LLNL. Research hydrogeologist working with numerical modeling of subsurface flow and transport problems. Primary involvement has been with groundwater remediation management. Currently Co-PI on two Work For Others projects: 1) Reservoir Management Under Uncertainty (funded by the Center for Marine & Petroleum Technology of the UK) and 2) Using Artificial Neural Networks and the Genetic Algorithm to Optimize Well-field Design (funded by British Petroleum on behalf of the DeepLook Consortium). Also supporting Yucca Mountain Introduced Materials Task using neural networks to examine biogeochemical interactions. Co-PI (1989-1990) on project to determine field-based retardation factors at LLNL. Also worked with unconventional gas reservoir modeling, field hydrogeology, unsaturated infiltration experiments, and land use planning programs.

1990-1996 **Remediation Optimization Team Leader-** Coordinated incorporation of hydrogeologic characterization and solute transport modeling into optimization of remedial pump-and-treat strategies at LLNL (using nonlinear programming, artificial neural networks, and the genetic algorithm). Responsible for the Team which ranged from 2-10 people and involved a peak annual budget of 800K.

1982-1986 **Geology Instructor-** Chabot Junior College, Hayward, CA. Taught geology classes.

1978-1979 **Hydrologic Technician-** Water Resources Division, US Geological Survey. Involved with numerical modeling and other research topics concerned with the Sheffield, Illinois low level radioactive waste site.

1977-1978 **Geology Teaching Assistant-** University of Illinois. Conducted laboratory and discussion sessions. Also taught field mapping techniques at U. of I. Summer Field Camp, Sheridan, Wyoming.

GENERAL RESEARCH INTERESTS:

Solving problems of groundwater flow systems, water quality, and management of groundwater remediation using intelligent technologies such as neural networks and heuristic nonlinear optimization techniques (genetic algorithms and simulated annealing). Expansion of these techniques into reservoir management for enhanced oil recovery.

PROFESSIONAL ACTIVITIES

¥ LLNL Site Coordinator for the DOE Environmental Restoration and Waste Management Fellowships

¥ Member of the University of California at Berkeley Initiative on Soft Computing (BISC) Special Interest Group on Earth Sciences

¥ Co-chair of LLNL Earth and Environmental Sciences Directorate Ombuds Program

¥ Visiting Scholar at Stanford University Petroleum Engineering Department Summer 1999

HONORS

¥ Who's Who in American Universities and Colleges, Mortarboard, University Scholar, Three Year Degree Student, Alpha Lambda Delta Sophomore Award (highest GPA), Kappa Mu Epsilon (math honorary), National Association of Geology Teachers Summer Field Course Scholarship.

PERSONAL:

Citizenship: USA

PROFESSIONAL MEMBERSHIPS:

¥ American Geophysical Union

¥ Geological Society of America

¥ Society of Petroleum Engineers

BOOK AND REFEREED JOURNALS SINCE 1992.

¥ Dowla, F.U. and L.L. Rogers, 1995. "Solving Problems in Environmental Engineering and the Geosciences with Artificial Neural Networks. MIT Press, Cambridge, MA, 239p.

¥ Rogers, L.L., F.U. Dowla, and V.M. Johnson, 1995. Optimal Field-Scale groundwater remediation using neural networks and the genetic algorithm, Environ Sci and Tech, Vol. 29, No. 5, pp: 1145-1155.

¥ Johnson, V.M and L.L. Rogers, 1995. Location analysis in ground-water remediation using neural networks. Groundwater, Vol. 33, No. 5, pp. 749-758.

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¥ Johnson, V.M. and L.L. Rogers. 1998. ÒUsing artificial neural networks and the genetic algorithm to optimize well-field design: Phase I Final Report.Ó Also Lawrence Livermore National Laboratory Report UCRL-ID-132280.

PUBLISHED ARTICLES IN CONFERENCE PROCEEDINGS SINCE 1990

¥ Rogers, L.L., V.M. Johnson, and R.B. Knapp, 1998. Remediation tradeoffs addressed with genetic algorithm-artificial neural network optimization. Proceedings of the XII International Conference on Compuational Methods in Water Resources, Greece, June 15-19, 1998. Also Lawrence Livermore National Laboratory UCRL-JC-129850, Livermore, CA.

¥ Rogers, L.L., V.M. Johnson, and W. Bosl, 1996. 3-D field-scale remediation optimization at Lawrence Livermore National Laboratory. EOS, Transaction, American Geophysical Union, 77(46)F267.

¥ Johnson, V.M., and L.L. Rogers, 1995. Poor man's parallelism in environmental management. Paper submitted to 2nd Congress on Computing in Civil Engineering Atlanta, Ga, June 5-7, 1995. Lawrence Livermore National Laboratory UCRL-JC-119732.

¥ Rogers, L.L., V.M. Johnson, and F. U. Dowla, 1994. Groundwater remediation management and artificial neural networks. Paper included in the Proceedings of the American Association for Artificial Intelligence Workshop: AI Technologies for Environmental Applications, Seattle, Washington July 31-August 4, 1994. (Invited)

¥ Johnson, V.M., and L.L. Rogers, 1994. Use of genetic algorithms and neural networks to optimize well locations and reduce well requirements. Paper included in the Conference Documentation of the Petroleum Science and Technology Institute Conference on Advances in Reservoir Technology, London, UK, November 7-8, 1994. (Invited).

¥ Rogers, L.L., V.M. Johnson, and F.U. Dowla, 1993. Network dissection of neural networks used in optimal groundwater remediation, Proceedings of the American Institute of Hydrology USA/USSR Second Joint Conference on Environmental Hydrology and Hydrogeology, Washington, D.C., May 16-21, 1993.

¥ Rogers, L.L., and F.U. Dowla, 1992. Groundwater remediation optimization with artificial neural networks and the genetic algorithm. EOS, Transactions, American Geophysical Union, 73(43);186.

¥ Johnson, V.M., L.L. Rogers, and F.U. Dowla, 1992. Application of artificial neural network technology to the optimization of field-scale pump-and-treat remediation. EOS, Transactions, American Geophysical Union, 73(43);234.

¥ Rogers, L. L., 1991 (October). Simulation-management methodology involving solute transport, nonlinear programming, and multiple management periods, Abstracts of the 1991 Geological Society of America Annual Meeting, p. 377.

¥ Rogers, L.L., 1990. Demonstration of incorporating sorption into nonlinear optimial remediation: principles and practical implications. Proceedings of the American Institute of Hydrology USA/USSR Joint Conference on Environmental Hydrology and Hydrogeology, Leningrad, U.S.S.R., June 18-21, 1990.

¥ Rogers, L.L., 1990. Time moment analyses of input to nonlinear simulation-management: sorption and formulation issues. EOS, Transactions, American Geophysical Union, 71(43);1335.

¥ Rogers, L L., D.W. Rice Jr., D.J. Bishop, and N.D. Stout. 1990. Cooperative LLNL/HAZWRAP project to demonstrate determination of field-based retardation factors: Part 3. algorithm to determine a field-based retardation factor. Proceedings for the Waste Management 1990 Conference in Tucson, Arizona, February 25-March 1, 1990.

¥ Jovanovich, M.C., R.A. Caufield, D.W. Rice,Jr, D.J. Bishop, and L.L. Rogers, 1990. Spatially discrete method for determining field-based sorption constants for volatile organic compounds. EOS, Transactions, American Geophysical Union, 71(43);1306.

¥ Rice, D.W. Jr., D.J. Bishop, and L.L. Rogers, 1990. Cooperative LLNL/HAZWRAP project to demonstrate determination of field-based retardation factors: Part 1. Distribution of Perchlorethylene around and within permeable zones in saturated alluvial deposits. Proceedings for the Waste Management 1990 Conference in Tucson, Arizona, February 25-March 1, 1990.
¥ Rice, D.W. Jr, M.C. Jovanovich, R.A. Caufield, D.J.Bishop, and L.L. Rogers, 1990. Displacement of saturated sediment pore water during rotary mud sampling. EOS, Transactions, American Geophysical Union, 71(43);1311.
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¥ Bishop, D.J., J.L. Sandoval, L.L. Rogers, D.W. Rice Jr., M. Reinhard, and E. McDonald, 1990. Sorption of volatile organic compounds (VOCs) in the saturated and unsaturated zones of a VOC-contaminated ground water site. EOS, Transactions, American Geophysical Union, 71(43);1301.

RECENT INVITED PRESENTATIONS:

¥ Society of Industrial and Applied Mathematics Workshop on Artificial Intelligence in Geophysics, June 15-17, 1997, Alburqurque, New Mexico.
¥ Los Alamos National Laboratory and Society of Industrial and Applied Mathematics Workshop on Mathematical Issues in Bioremediation, June 11-13, 1997, Los Alamos, New Mexico.